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Kinetics of low temperature dislocation plasticity in a refractory multi-principal element alloy

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ABSTRACT

A rigorous identification of the temperature-dependent, rate-controlling dislocation mechanisms and their associated kinetics in refractory multi-principal element alloys (RMPEAs) is fundamental to the development of predictive strengthening frameworks. In this work, we isolate single-slip {110}<111> plasticity in the BCC RMPEA $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$ (at.%) using orientation-controlled micropillar compression between 200–300 K and strain rates from 10^{-3} to 10^2 s^{-1} . The adherence to a single-slip condition enables direct determination of the temperature and strain-rate dependence of the critical resolved shear stress and the associated activation parameters. By combining transmission electron microscopy, phase-field dislocation dynamics (PFDD) simulations, and analytical strengthening models, the governing dislocation-mediated plasticity mechanism and its temperature evolution are identified. The results establish the rate-limiting role of screw dislocations, quantify the relative mobility of edge and screw segments, and assess the predictive capability of existing analytical models. The convergence between experiments, theoretical models and PFDD simulations provides a mechanistically consistent framework for understanding temperature-dependent plasticity in chemically complex BCC alloys and advances the development of physics-based strengthening descriptions for RMPEAs.

1. Introduction

Refractory multi-principal element alloys (RMPEAs), particularly those characterized by single-phase body-centered cubic (BCC) solid solutions, have attracted sustained interest as candidate materials for structural applications in extreme environments [1]. Their exceptionally high melting temperatures, strength retention at elevated temperatures, and resistance to diffusion-controlled degradation position them favorably for aerospace propulsion systems, nuclear technologies,

and space infrastructure [2–8]. These unique property combinations arise from chemical complexity that introduces spatially fluctuating local energy barriers, fundamentally altering dislocation behavior relative to dilute BCC metals [1,9]. Crucially, the same dislocation-level mechanisms responsible for exceptional high-temperature strength also exhibit a pronounced temperature-dependent behavior, influencing not only strength but also toughness, e.g., the transition from brittle fracture to ductile flow [10–13]. This sensitivity directly impacts the room-temperature formability, manufacturability, and broader applicability

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of RMPEAs, making an understanding of dislocation motion from cryogenic to high temperatures essential for assessing mechanical reliability.

Low temperature plastic deformation in BCC metals is governed predominantly by screw dislocation mobility, where glide is significantly hindered by lattice friction associated with the Peierls potential [14,15] due to complex core arrangements. In pure and dilute BCC systems, screw dislocation motion proceeds via thermally activated kink-pair nucleation and migration, resulting in strong temperature and strain-rate sensitivity of the critical resolved shear stress [16,17]. This mechanism underlies characteristic features of BCC plasticity, including the rapid increase in flow stress with decreasing temperature, non-Schmid effects, and tension–compression asymmetry [18–30]. Edge dislocations, in contrast, experience substantially lower lattice resistance and therefore exhibit much higher mobilities, and thus are not rate-limiting under most conditions [31–34].

In RMPEAs, this classical picture is substantially modified [35]. Pronounced chemical disorder and the resulting lattice distortions alter dislocation core structures and reshape the energetic landscape governing dislocation glide for screw and edge dislocations [36–41]. Atomistic simulations have shown that screw dislocations in RMPEAs can adopt intrinsically kinked configurations driven by local compositional fluctuations, such that motion becomes limited by kink migration rather than kink-pair nucleation [37,41–44]. In addition, chemically induced cross-kinking has been identified as a key contributor to the elevated strength and work-hardening behavior of these alloys. Phenomena such as extensive cross-slip on non-primary slip planes, thermally activated superjogs, and the sluggish mobility of edge dislocations [45–49], comparable to that of screws in certain compositions, also play pivotal roles in dictating the mechanical response, especially at elevated temperatures. These considerations suggest that the identity of the rate-controlling dislocation character may depend sensitively on both composition and temperature.

To rationalize these observations, several analytical models have been developed to describe the temperature-dependent strength of RMPEAs by explicitly accounting for the interaction between dislocations and their chemically disordered environment. Two predominant frameworks have emerged. One class of models, initially advanced by Suzuki [50] and later readapted by Rao [51] emphasizes screw dislocation-controlled plasticity. In this picture, short-range solute interactions dominate the resistance to motion. The second class of models, introduced by Maresca and Curtin [36], assumes edge dislocation-controlled plasticity, in which glide resistance arises from long-range elastic interactions between the dislocation stress field and spatially varying solute-induced misfit volumes. Here, deformation is thought to proceed through the thermally activated depinning of dislocation segments from a heterogeneous elastic landscape. While both models have shown good agreement with the strength–temperature trends of some RMPEA compositions, each presupposes the rate limiting glide mechanism and constructs its analytical solution accordingly. Despite reports on the dislocation behavior in RMPEAs [42,45,47,52,53], no concrete experimental evidence has validated the operative deformation mechanism asserted by either model and quantified the kinetics of both screw- and edge-type dislocations in the same system. From a fundamental perspective, the low temperature plasticity regime (homologous temperature $T/T_m < 0.2$, where T_m is the melting temperature) is of particular interest, where small differences in activation energies can lead to pronounced variations in strength and flow behavior [9]. Low temperature investigations thus provide a uniquely sensitive experimental window in which intrinsic dislocation mechanisms dominate the mechanical response.

In this work, we investigate the compressive plasticity of a single-phase RMPEA, $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$. This non-equiatomic composition was selected through a theory-guided alloy design strategy aimed at achieving high melting temperature, thermodynamic stability, and robust deformation resistance, while suppressing the formation of

hexagonal close-packed (HCP) precipitates observed in the equiatomic HfNbTiTaZr refractory alloy [1,12]. Moreover, previous investigations on similar compositions in the Hf-Mo-Nb-Ta-Ti system have shown RMPEAs with sustained yield strength over a broad temperature range [54], melting temperatures > 2300 K, and moderate densities ($> 8 \text{ g/cm}^3$) [55], positioning this alloy system as a highly promising candidate for future research and structural applications [6,7]. We focus on single crystals to avoid the confounding effects of grain boundaries, crystallographic texture, and heterogeneous stress states in the interpretation of dislocation glide mechanisms. Here, single-crystal micropillar compression experiments are performed across cryogenic and ambient temperatures, from ~ 200 to 300 K. The micropillar geometry, combined with a crystallographic orientation selected to promote activation of the primary $\{110\}\langle 111 \rangle$ slip system, enables direct interrogation of dislocation glide while avoiding extrinsic effects associated with grain boundaries and microstructural heterogeneity. Although RMPEAs are primarily targeted for elevated-temperature applications, the low-homologous-temperature regime is deliberately examined here because it maximizes sensitivity to thermally activated lattice resistance and enables the intrinsic rate-controlling glide mechanisms of the single-phase solid solution to be isolated. Establishing these elementary processes provides a mechanistic baseline for interpreting their competition with additional thermally activated deformation mechanisms and microstructural evolution that may emerge at higher temperatures.

2. Materials and methods

2.1. Sample preparation

A 40 g button with the composition $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$ (at.%) was arc melted from pure elements (Nb foil, Ti foil, Ta plate, Hf turnings, and Mo pellets). All constituent elements had a purity of 99.7% or higher and were layered according to their melting point. Arc-melting occurred on a water-cooled copper hearth under an Ar atmosphere; a Ti getter adjacent to the sample was melted prior to each melting step. The RMPEA button was flipped and remelted four times to ensure homogeneity.

Sections cut from the samples were annealed in a Vacuum Industries Hot Press at 1500°C for 24 h to promote chemical homogenization. The corresponding phase diagram for this alloy composition, calculated using the CALPHAD method [56], is presented in Figure S.1 of the Supplementary Materials. From this diagram, a melting temperature T_m of 2475 K was estimated for the $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$ alloy. To mitigate oxidation during annealing, the specimens were wrapped in Ta foil and encapsulated within sealed Ta ampules. Foils made of Ti were placed adjacent to the samples to serve as oxygen-getters. The annealing was performed under vacuum conditions maintained below 200 mTorr . Upon completion, the samples were cooled at the maximum rate permitted by the furnace, with an estimated peak cooling rate of approximately $45^\circ\text{C min}^{-1}$.

2.2. Chemical and microstructure characterization

Wavelength-dispersive X-ray fluorescence (WDXRF) measurements of the bulk alloy compositions were conducted with a Rigaku ZSX Primus IV and are presented in Table 1. Interstitial contents were also measured by inert gas fusion (O and N) and combustion analysis (C), both performed by Northern Analytical, Inc.

To prepare the material for subsequent analysis, the surface perpendicular to the through-thickness direction was ground down using 1200 grit SiC papers and mechanically polished from 15 to $0.1 \mu\text{m}$ using diamond suspension. The surface was further polished in a solution of colloidal silica ($0.05 \mu\text{m}$) on a Vibromet vibratory polisher (Buehler, Lake Bluff, IL, USA). Final cleaning was carried out using ethanol, followed by de-ionized water and drying in air.

Table 1

Alloy composition measured using WDXRF, inert gas fusion (O and N) and combustion analysis (C).

Hf (at.%)	Mo (at.%)	Nb (at.%)	Ta (at.%)	Ti (at.%)	Oxygen (ppmw)	Nitrogen (ppmw)	Carbon (ppmw)
10.1	9.8	34.7	20.0	25.4	401	44	59

Electron backscattered diffraction (EBSD) maps of the polished surface were collected and recorded for subsequent analyses using an EDAX DigiView camera installed on a Thermo Fisher Scientific Apreo-C scanning electron microscope (SEM). Each map was acquired with 2×2 binning, electron beam conditions of 20 kV and 13 nA (beam diameter of ~ 10 nm), sample tilt 70° , and a step size of $0.5 \mu\text{m}$.

A total of 44 micro-pillars, nominally identical in geometry (diameter of $5 \mu\text{m}$; height of $10 \mu\text{m}$) and orientation, were fabricated using a FEI Helios Dualbeam Nanolab 600 focused ion beam (FIB)-SEM. The aspect ratio of height to diameter of 2:1 was selected to prevent buckling. The pillar taper, caused by inherent limitations of the FIB milling procedure, was found to be on average $1\text{--}2^\circ$ and the surfaces showed negligible curtaining artifacts.

2.3. Mechanical testing and post-deformation characterization

Micropillar compression was conducted using the in situ Alemnis microindenter module (Alemnis AG, Switzerland), previously employed for elevated temperature experiments [57,58], but modified for cryogenic conditions, within a DSM 962 SEM (Zeiss, Germany) [59,60]. Two configuration designs were implemented to allow for quasi-static and high-strain rate testing [61,62]. For the former, the load was measured using a strain gauge-based load cell which yields reliable measurements for low strain rates ($\leq 1 \text{ s}^{-1}$), while for the latter, a piezoelectric load cell was used for strain rates $\geq 1 \text{ s}^{-1}$. The principal components of the cryogenic unit have been described in earlier works [59,63]. A cold finger, connected to both the sample and tip holders by copper braids, is cooled by nitrogen circulated from a 25 L dewar positioned outside the vacuum chamber. Following thermal stabilization, thermocouples embedded in the tip and sample holders recorded a baseline temperature of 113 K. Independent thermal control of the indenter and sample was employed to minimize temperature gradients and associated drift. Localized cooling, thermal isolation of the cold regions, and a closed-loop frame temperature regulation system effectively reduced frame drift, noise, and the need for temperature-dependent calibration. The frame compliance was determined to be 4.96 nm/mN for quasi-static and 5.18 nm/mN for high-strain rate conditions by unloading stiffness measurements from multiple indents on fused silica, according to the method in [64].

The tests were conducted in displacement-controlled mode. A wide range of strain rates were applied spanning five orders of magnitude, from 10^{-3} to 100 s^{-1} . The maximum achievable strain rate in these tests is primarily limited by the maximum actuation speed of the in situ dynamic nano-indentation system (1 mm/s) and the dimensions of the micropillars. In the present study, with a pillar height of $10 \mu\text{m}$, strain rates of approximately 100 s^{-1} were attainable. Measurements of the actual sample surface (test) temperatures were performed using a thermocouple in contact with the sample surface. Testing was realized at three different surface temperatures: 206 ± 1 , 232 ± 2 , and $300 \pm 2 \text{ K}$. The temperature value of 206 K represents the lowest sample surface temperature attainable, limited by thermal losses across the sample thickness. For quasi-static compressions ($\leq 1 \text{ s}^{-1}$), thermal drift was minimized at each temperature by ensuring the matching of the tip and sample surface temperatures, according to the method outlined in Ref. [65]. The maximum allowable drift rate was chosen as 1 nm/s .

The specimens were compressed with a nanoindenter fitted with a $20 \mu\text{m}$ diameter WC flat punch (Synton-MDP, Switzerland). The engineering stress σ was calculated using the cross-sectional area measured at the mid-height of the pillar. Stresses, σ and τ , and strain ϵ are nominal. The compliance of the pillar geometry is considered by applying

Sneddon's and Zhang's corrections [66] during yield strength calculations using the associated MicroMechanics Data Analyzer (MMDA) software. Of the 44 pillars, 40 were designated for mechanical testing under various loading conditions. For statistical reliability, two or more pillars were tested for each experimental condition (T , ϵ). To enable post-mortem analysis of different stages of plastic deformation, distinct strain levels were intentionally applied at each loading condition. Note that both quasi-static and high-strain rate systems were employed to deform pillars at a strain rate of 1 s^{-1} , enabling a fair comparison of stress values measured using strain-gauge-based and piezoelectric load cells, thereby confirming consistency and ensuring compatibility across the entire strain-rate spectrum investigated.

After deformation, an electron transparent lamella foil was extracted along slip traces from a deformed pillar, with the last thinning step performed at 5 keV and 100 pA. Transmission electron microscopy (TEM) imaging was performed using conventional TEM and scanning (S/)/TEM modes on a Spectra 200 probe aberration-corrected S/TEM equipped with an S-CORR corrector and a cold field-emission gun (X-CFEG), as well as on a Talos F200X equipped with Chemi STEM EDS (Thermo Fisher Scientific). Samples were evaluated at 200 keV using collection angles of 9 mrad (bright field images) and $61\text{--}200 \text{ mrad}$ (high-angle annular dark field, HAADF).

2.4. Simulations

Molecular dynamics (MD) and phase-field dislocation dynamics (PFDD) simulations were conducted. All atomistic quantities used as model inputs were calculated assuming an ideal random solid solution at the experimentally measured alloy composition. The material parameters derived from the MD simulations for $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$ are summarized in Table 2, while the simulation details are reported in Section A.1 of Appendix A. PFDD simulations are used to predict the onset and evolution of plastic deformation in single crystal $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$. A detailed account of the PFDD model and its numerical implementation can be found in [67–69]. Below, we describe the PFDD setup and inputs.

PFDD models dislocation-mediated plasticity in crystals through a continuum, energy-based framework that uses phase-field order parameters to track slip on crystallographic planes. A three-dimensional, non-orthogonal BCC computational grid is employed. Grid points of volume Ω coincide with BCC lattice sites [71]. Each slip system α is represented by an order parameter ϕ^α that evolves to drive the crystal toward its lowest free-energy configuration. The spatiotemporal evolution of ϕ^α follows a stochastic time-dependent Ginzburg–Landau equation:

$$\phi^\alpha(\mathbf{r}, t) = -L \frac{\delta \psi_\Omega[\{\phi\}]}{\delta \phi^\alpha(\mathbf{r}, t)} + \theta(\mathbf{r}, t) \quad (1)$$

Here, $\mathbf{r}$ and t indicate the spatial position vector and time, respectively. L sets the timescale for system relaxation toward a local free energy minimum. The free energy density ψ_Ω combines contributions from applied stress, elastic strain energy, and lattice potential. The Langevin noise term θ introduces stochastic fluctuations that mimic thermal perturbations to the dislocation configuration.

We construct a BCC simulation cell of the $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$ RMPEA. The variable energy barriers that arise from the chemical disorder are assigned to all (110) planes using the workflow described in [72]. The barriers are calculated via MD, and hence reflect the dependence on local composition, atomic configuration, and lattice distortion (Section A.1 of the Appendix). Dislocations are placed in the central (110) plane, and deformation simulations are carried out at

Table 2

Lattice parameter a and elastic constants C_{11} , C_{12} , C_{44} of the constituent elements and of the alloy. The values of the constituent elements are taken from [70] while those for the alloy are obtained via MD simulations as described in Section A.1 in the Appendix. The elastic constants are used to calculate the shear modulus μ_{V-R} , bulk modulus B , and Poisson's ratio ν . The shear modulus is calculated using the Hill approximation (Voigt-Reuss average). These values are used in Section 4.1 to estimate the critical resolved shear stress of the alloy, τ_{CRSS} , from the screw/edge strengthening theories [36,51].

Material (BCC)	Hf	Mo	Nb	Ta	Ti	Hf ₁₀ Mo ₁₀ Nb ₃₅ Ta ₂₀ Ti ₂₅ (0 K)	Hf ₁₀ Mo ₁₀ Nb ₃₅ Ta ₂₀ Ti ₂₅ (300 K)
a [nm]	0.3558	0.3144	0.3299	0.3301	0.3264	0.3303	0.3309
C_{11} [GPa]	131	450	253	266	134	206.99	203.02
C_{12} [GPa]	103	173	133	158	110	131.09	127.76
C_{44} [GPa]	45	125	31	87	36	69.89	68.53
μ_{V-R} [GPa]	28.2	130.2	40.5	71.8	23.2	54.7	53.9
B [GPa]	112.3	265.3	173.0	194.0	118.0	156.4	152.8
ν	0.384	0.289	0.391	0.335	0.408	0.34	0.34

temperatures T of 200, 230 and 300 K, in line with the experimental temperatures. Periodic boundary conditions are applied in all three directions.

A constant shear stress τ^{app} is applied, resolved only on the active slip system. Dislocations evolve under these loading and thermal conditions for a specified number of timesteps. Based on evidence that screw dislocation glide limits rate behavior at low temperatures in BCC alloys, long screw dislocations are explicitly modeled to isolate their contribution to RMPEA deformation. Dislocation loop expansion is also simulated to evaluate the kinetics of edge-, mixed-, and screw-segment contributions to low-temperature deformation.

Screw Dipole Configuration: A screw dipole is initialized on the habit plane at the center of a $128b \times 128b \times 128b$ cell with a $64b$ separation. This dipole remains stable under zero applied stress. In the stress-free configuration, each dislocation core spreads onto all three $\{110\}$ planes intersecting the $\langle 111 \rangle$ line. Due to atomic-scale chemical disorder, dislocations in RMPEAs can exhibit jerky, intermittent motion below critical stress thresholds [73]. To examine continuous glide, we identify the threshold stress τ^d as the minimum stress required to drive the screw dislocation over a long distance of approximately $20b$ within a defined timestep. This is achieved by incrementally increasing τ^{app} by $\Delta\tau = 0.0001\mu$ (with μ the shear modulus obtained from Table 2). By enforcing this uniform displacement (and hence strain) threshold, direct comparisons of τ^d as a function of temperature and strain rate become physically meaningful, and the calculated values reflect the intrinsic stress required to sustain steady-state dislocation glide at a given thermodynamic state.

The critical stress τ^d is determined at six constant strain rate conditions: $\dot{\epsilon}^d = 0.01, 0.02, 0.05, 0.1, 1, \text{ and } 2 \text{ s}^{-1}$. The plastic strain tensor is computed from the slip order parameters as:

$$\epsilon_{ij}^p = \frac{1}{2} \sum_{\alpha=1}^N \frac{b^\alpha \phi^\alpha}{d^\alpha} \left(s_i^\alpha n_j^\alpha + n_i^\alpha s_j^\alpha \right) \quad (2)$$

Here, N is the number of slip systems. For each α , s^α and n^α are the unit slip direction and plane normal, respectively; d^α is the interplanar spacing, and b^α is the Burgers vector magnitude. The von Mises equivalent plastic strain is computed as:

$$\bar{\epsilon}_{eq}^p = \frac{1}{\Omega} \int_{\Omega} \sqrt{\frac{2}{3} \epsilon_{ij}^p \epsilon_{ij}^p} d\Omega \quad (3)$$

The strain rate $\dot{\epsilon}^d$ is then approximated as:

$$\dot{\epsilon}^d \approx \frac{\bar{\epsilon}_{eq}^p}{\Delta t \cdot n_t} \quad (4)$$

where Δt is the timestep size and n_t is the number of timesteps over which strain accumulates.

Dislocation Loop Configuration: A circular dislocation loop with initial radius $16b$ is placed on the habit plane at the center of a $256b \times 256b \times 256b$ cell. This loop is stable under zero applied stress and expands under applied temperature T and τ^{app} . Screw segments lie parallel to the Burgers vector $\mathbf{b}$, edge segments lie perpendicular to $\mathbf{b}$, and remaining segments exhibit mixed character.

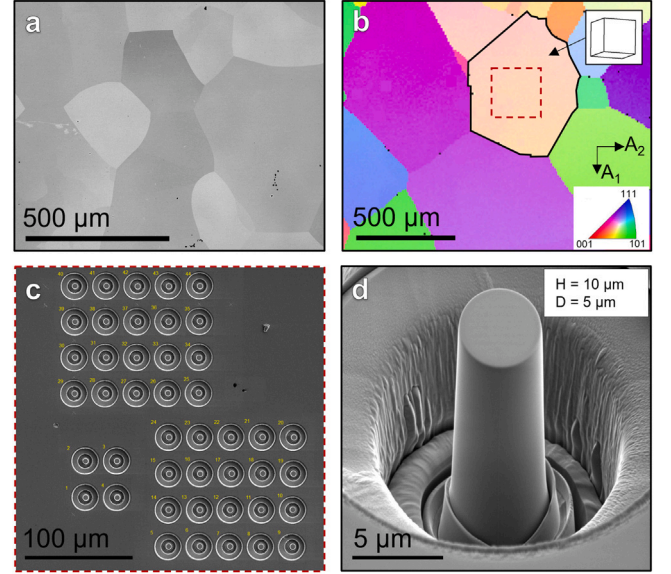


Fig. 1. Overview of the microstructure and site-specific micro-pillar fabrication. (a) Secondary electron (SE) image of the sample after homogenization treatment. (b) EBSD Inverse Pole Figure (IPF) map of a selected region of the sample, with the grain chosen for micro-pillar fabrication outlined by a solid black line. The selected grain has Euler angles (Bunge convention) of $\phi_1 = 89.8^\circ$, $\Phi = 81.7^\circ$, and $\phi_2 = 67.4^\circ$. (c) Overview of the array consisting of 44 micro-pillars fabricated via FIB. (d) High-magnification SE image of a representative micro-pillar.

Table 3

Maximum Schmid factor, m_{SF} , associated with each candidate BCC slip-system (S.S.) family for the selected single-crystal loading orientation.

S.S.	$\{110\}\langle 111 \rangle$	$\{112\}\langle 111 \rangle$	$\{123\}\langle 111 \rangle$	$\{134\}\langle 111 \rangle$
m_{SF}	0.499	0.433	0.472	0.484

3. Results

The synthesis and homogenization procedures produced a single-phase microstructure with equiaxed, polygonal grains of relatively large size (Fig. 1a and 1b). EBSD did not reveal preferential texture and the average grain size was measured to be $523 \pm 58 \mu\text{m}$. A single grain, outlined in black in Fig. 1b, was selected for the fabrication of micro-pillars. This grain was deliberately chosen to maximize the Schmid factor, m_{SF} , associated with the $\{110\}\langle 111 \rangle$ slip system (Table 3). An overview of the array of 44 micro-pillars, fabricated with nominally identical geometry and orientation, is presented in Fig. 1c, while a representative image of an individual undeformed pillar is shown in Fig. 1d.

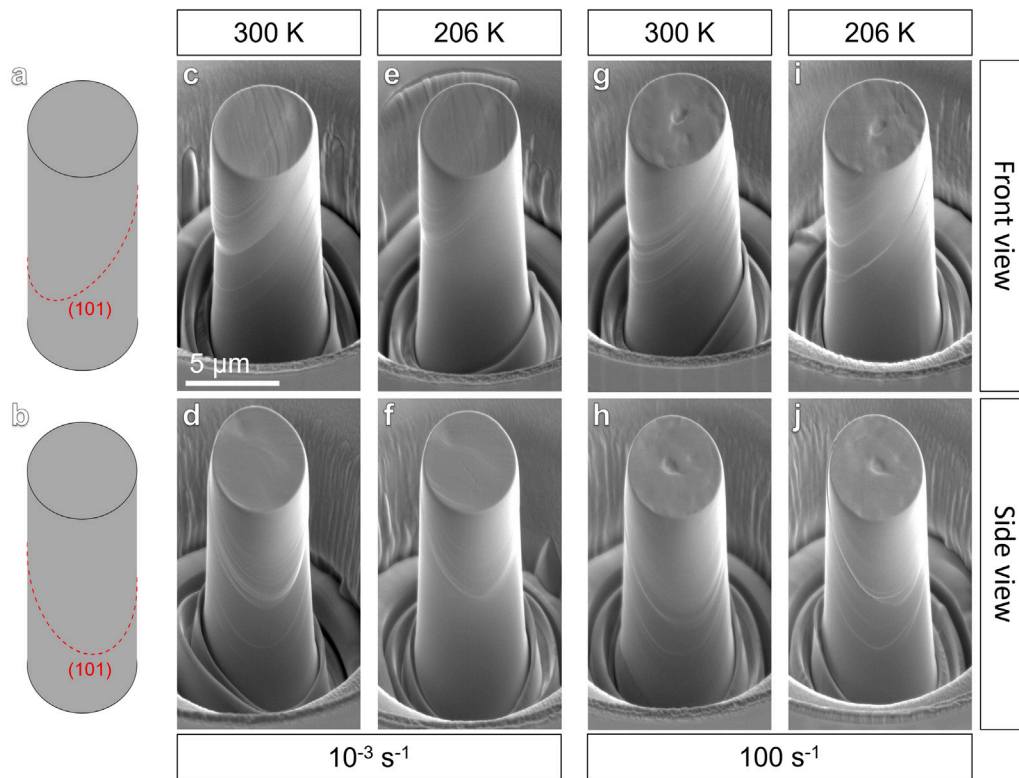


Fig. 2. SE images of micro-pillars deformed to a comparable total strain value ($\sim 8 \pm 1\%$) at 206 K and 300 K under strain rates of 10^{-3} and 100 s^{-1} , showing single-slip behavior. The SE images are tilt corrected as they are acquired from a 45° tilt. Slip trace analysis, aided by EBSD-based crystallographic orientation data and MTEX simulations (a,b), confirms activation of the (101) slip plane in all cases (c-j).

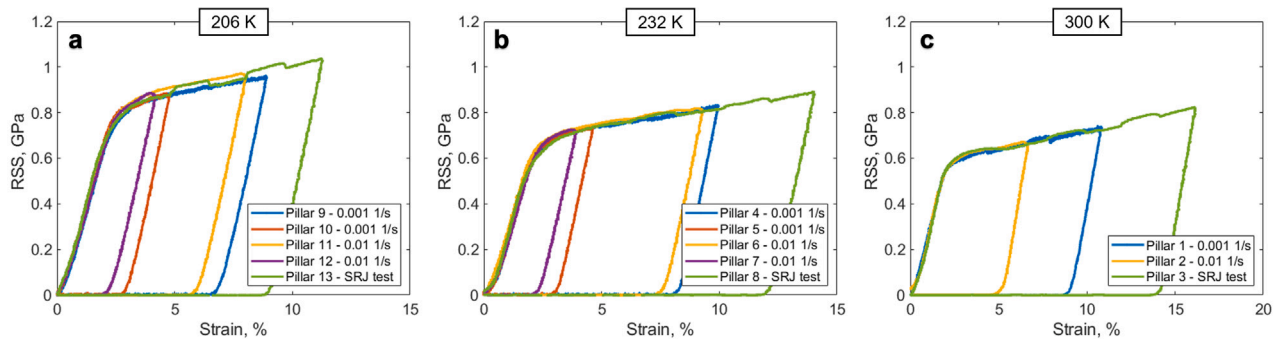


Fig. 3. Stress-strain curves at the different temperatures and for strain rates of 10^{-3} and 10^{-2} s^{-1} . The strain is the nominal engineering strain ϵ . In the legend, “SRJ” denotes pillars deformed by the strain rate jump (SRJ) method.

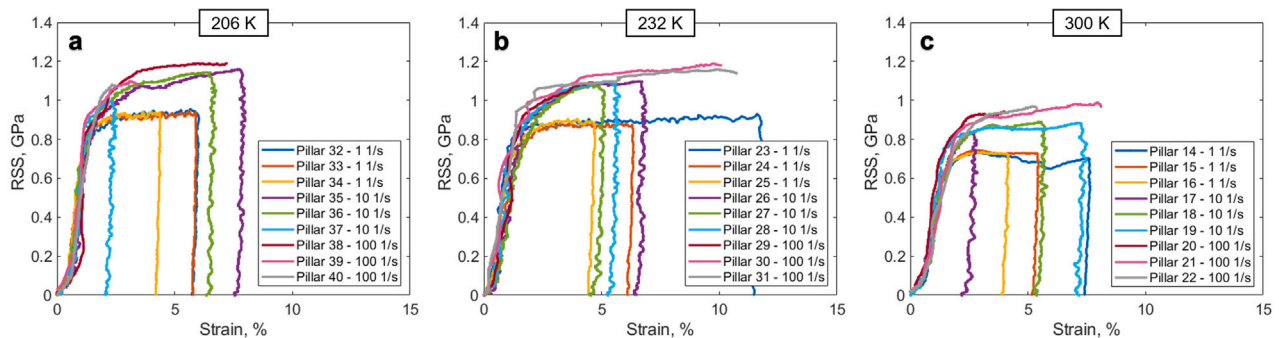


Fig. 4. Stress-strain curves at the different temperatures and for strain rates of 1, 10, and 100 s^{-1} . The strain is the nominal engineering strain ϵ . Note that at strain rates of 10 and 100 s^{-1} , the raw material response is significantly affected by oscillatory noise, precluding an accurate determination of its mechanical properties. To mitigate this effect, an adjacent averaging procedure over every 50 data points was implemented. For reference, the experimental data under these conditions were acquired at a sampling rate of 1 MHz. Accordingly, higher uncertainties have been accounted for in evaluating the response and extracting CRSS values.

Following deformation across the entire range of temperatures and strain rates, the activation of a single slip system was exhibited, as evidenced by slip traces on the micro-pillar surfaces (the extreme bounds of temperatures and strain rates are shown in Fig. 2). To precisely identify the active slip plane, a custom MATLAB routine based on the MTEX crystallographic toolbox was employed [74], which utilizes EBSD-derived crystallographic orientation data to project candidate slip planes onto the surfaces of virtual micro-pillars (Fig. 2a and 2b) acquired from multiple imaging perspectives (see Section S.2 of the Supplementary Materials). This procedure is adapted from prior micro-pillar studies on similar BCC alloys [52,75–78]. Despite the known complexities associated with slip trace analysis in BCC metals where surface features can deviate from the traces of single crystallographic planes or exhibit non-planar characteristics [23,30,52,79], it was found that all deformation-induced traces here were consistently attributable to a single crystallographic plane, namely the (101)⁽⁶⁾.

Furthermore, Fig. 2 reveals a noticeable strain rate dependence in the spatial distribution of slip traces along the micro-pillars. At the lowest applied strain rate of 10^{-3} s^{-1} (Fig. 2c–f), plastic deformation is predominantly localized near the top region of the pillar, in the vicinity of the flat punch contact interface. This region is thought to experience the highest stress concentration due to its direct contact with the indenter and the associated mechanical constraint imposed by the contact boundary conditions. The observed clustering of slip traces in this zone (Fig. 2c) suggests that dislocation motion is strongly influenced by the local stress gradient. The slip activity appears to initiate at or near the free surface at the pillar's top circumference and propagates downward, consistent with time-dependent dislocation nucleation/activation and motion concentrated at sites of maximal resolved shear stress. In contrast, under the higher applied strain rate of 100 s^{-1} (Fig. 2g–j), the distribution of slip traces becomes markedly more diffuse and shifts toward the midsection of the pillar. The absence of dominant slip initiation near the punch–pillar interface suggests that deformation is not limited to surface-initiated dislocation mechanisms but involves dislocation activity within a broader volume of the pillar, likely due to the limited time for dislocation interactions to concentrate in high-stress regions. This observation reflects the inherently rate-sensitive nature of dislocation mobility.

3.1. Mechanical response

The engineering stress–strain curves characterizing the mechanical response of the micro-pillars across the investigated range of temperatures and strain rates are presented in Fig. 3 for quasi-static and in Fig. 4 for high-strain rate compression. For brevity, tests conducted at strain rates below 1 s^{-1} are denoted as *quasi-static*, while those performed at strain rates equal to or exceeding 1 s^{-1} are referred to as *high-strain rate* tests. Notably, across all testing conditions, the curves exhibit a high degree of reproducibility, attesting both the reliability of the experimental method and the consistency of the underlying mechanisms governing plastic deformation behavior. In all cases, the stress reported corresponds to the resolved shear stress (RSS, $\tau_{\text{RSS}} = \sigma \cdot m_{\text{SF}}$) component for (101) slip.

The influence of temperature and strain rate on τ_{CRSS} is shown in Fig. 5, with values extracted at 1.5% total strain from the corresponding curves shown in Figs. 3 and 4. At any given strain rate, a pronounced increase in τ_{CRSS} is observed with decreasing temperature, consistent with a thermally activated plasticity mechanism in which dislocation motion becomes progressively more difficult at lower temperatures, as discussed in later sections. Additionally, for each temperature, τ_{CRSS} rises systematically with increasing strain rate (Fig. 5).

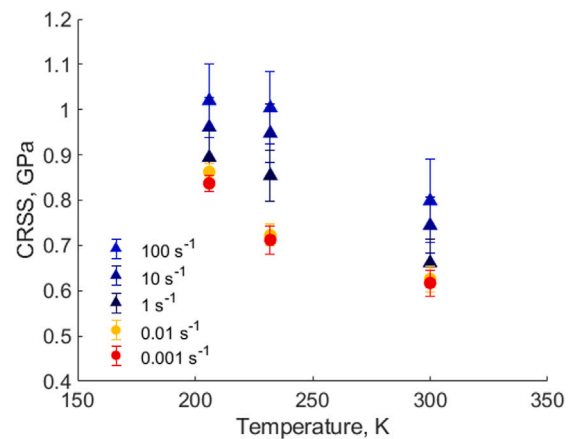


Fig. 5. Dependence of the critical resolved shear stress τ_{CRSS} on temperature and strain rate. The values of τ_{CRSS} are extracted from each curve in Figs. 3 and 4 at 1.5% strain. The mean and standard deviation for each condition are obtained by combining the means and variances of the critical stress values associated with the pillars deformed under the respective experimental conditions. Note that the error bars consider also uncertainties ($\pm 100 \text{ nm}$) in the measurements of the pillar dimensions. Circles correspond to quasi-static conditions, whilst triangles correspond to high-strain rate loading.

Unlike the responses typically observed in smaller micro-pillar specimens [80,81], all the stress–strain curves exhibited a smooth and continuous profile, with no signs of serrated flow or sudden load drops, indicating a deformation behavior akin to bulk-like plasticity. To compare the post-yield hardening response across temperatures under the same quasi-static loading condition, a representative engineering stress–strain curve at each test temperature, obtained at a nominal strain rate of 10^{-3} s^{-1} , was transformed into a true stress–strain curve and the corresponding work-hardening rate ($\Theta = d\tau_{\text{true}}/d\epsilon_{\text{true}}$) was computed (Fig. 6). The work-hardening rates converge to approximately 4000 MPa above 4% true strain, indicating a similar post-yield hardening response across the investigated temperatures under quasi-static loading. Importantly, because deformation under quasi-static conditions is spatially localized near the upper portion of the pillars, the same analysis was applied to the 100 s^{-1} experiments, for which deformation is substantially more diffuse along the pillar length. The resulting work-hardening rates are of comparable magnitude (see Fig. A.1 in Section A.2 of Appendix A). This indicates that the material response measured under quasi-static loading is not a consequence of localization near the pillar top, and that the extracted work-hardening rate reflects the intrinsic hardening response associated with plastic deformation along the $\{110\}\langle 111 \rangle$ slip system in the BCC RMPEA investigated here. This further suggests that, while the stress required to sustain plastic flow is rate dependent, the incremental hardening response per unit strain is much less rate dependent.

As micro-pillars with diameters of approximately $5 \mu\text{m}$ are sufficiently large to facilitate extensive dislocation–dislocation interactions characteristic of bulk-like plasticity, yet small enough to potentially experience size-dependent strengthening effects [82–85], we estimated the contribution of size effects on the measured τ_{CRSS} using a single-arm dislocation source model that has been successfully applied to other BCC refractory systems [82]. Specifically, using a lattice parameter of 0.33 nm (see Table 2), a corresponding Burgers vector magnitude b of 0.286 nm , an initial dislocation density $\rho_{d,0}$ of 10^{12} m^{-2} , a pillar diameter of $5 \mu\text{m}$, an aspect ratio of 2, a slip plane oriented at an angle $\beta = 45^\circ$ from the compression axis, and a shear modulus μ of 54 GPa (see Table 2), the estimated increase in τ_{CRSS} for the (101) slip system due to geometrically constrained source operation is $\sim 11 \text{ MPa}$. Because of the choice of a low initial dislocation density, this value should be regarded as an upper bound for the size effect and accounts for less

⁶ The lattice coordinate system used to define the Miller indices is reported in Fig. 8c.

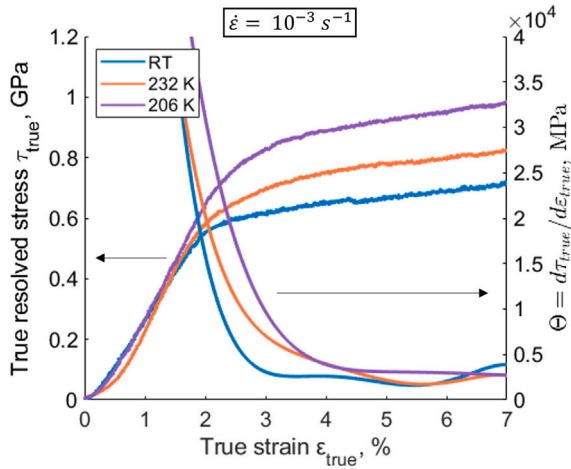


Fig. 6. True stress–strain curves and corresponding work-hardening rates ($\theta = d\tau_{\text{true}}/d\epsilon_{\text{true}}$) derived from representative engineering stress–strain data at each test temperature, measured at a nominal strain rate of 10^{-3} s^{-1} .

than 2% of the lowest measured τ_{CRSS} (i.e., 616 MPa at $T = 300 \text{ K}$ and a strain rate of 10^{-3} s^{-1}); thus, size effects can be considered negligible in influencing the yield behavior.

3.2. Activation parameters

Strain rate sensitivity m and apparent activation volume V_{app}^* are extracted from the temperature- and strain rate-dependent deformation behavior (Fig. 5), providing insight into the underlying thermally activated dislocation mechanisms governing plasticity. Specifically, m and V_{app}^* can be defined as:

$$m = \left. \frac{\partial \ln \tau}{\partial \ln \dot{\epsilon}} \right|_T \quad V_{\text{app}}^* = k_B T \left. \frac{\partial \ln \dot{\epsilon}}{\partial \tau} \right|_T \quad (5)$$

Under quasi-static loading, the strain rate sensitivity decreases with increasing temperature (Fig. 7a), with a substantially larger change between 206 and 232 K than between 232 and 300 K. This variation is consistent with a transition in the underlying thermally activated deformation mechanism, as discussed in Section 4.2. In parallel, the apparent activation volume increases progressively with temperature ranging from $\sim 11 \text{ b}^3$ at 206 K to $\sim 47 \text{ b}^3$ at 300 K (data are provided in Table S.1 in the Supplementary Materials). Under high-strain rate loading, in spite of the additional mechanical noise present in these measurements (Fig. 4), the strain rate sensitivity value increases compared to the quasi-static loading case in a statistically significant way, accompanied by a reduction in V_{app}^* (Fig. 7b). This will be discussed further in Section 4.2.

The activation parameters reported thus far correspond to τ_{CRSS} values extracted at 1.5% of total strain from independent pillars tested at constant-strain-rate. To assess the strain dependence of the rate response and to provide an internal check on the activation parameters obtained from these independent pillars, quasi-static strain-rate-jump (SRJ) tests were performed at each temperature. Each analyzed jump consisted of a change in strain rate from 10^{-3} to 10^{-2} s^{-1} and subsequently back to 10^{-3} s^{-1} , with these jumps repeated at different strain levels within the same pillar. Because the stress immediately before and after each jump is measured within the same pillar at essentially the same strain and geometry, the corresponding stress increment ($\Delta\tau_{\text{CRSS}}$) minimizes uncertainties associated with pillar-to-pillar variations in cross-sectional dimensions. Notably, the resulting stress–strain responses exhibit strong agreement with those obtained from independent tests performed at constant strain rates (Fig. 3), thereby providing

an internal validation of the rate dependence obtained from independent constant-strain-rate tests. For each temperature, the value of $\Delta\tau_{\text{CRSS}}$ remains essentially invariant across different strain values (Table 4). This invariance implies that the hardening response is comparable at both strain rates and that, consequently, the activation parameters do not exhibit sensitivity to strain, at least within the quasi-static regime and for the temperature range examined⁽⁷⁾. The strain-independence of these parameters strongly suggests that the underlying rate-controlling deformation mechanism remains unaltered throughout the investigated strain interval (i.e., up to $\sim 14\%$ of total strain). Moreover, as previously mentioned, the values of $\Delta\tau_{\text{CRSS}}$ also exhibit a systematic increase in magnitude with decreasing temperature, confirming that the strain-rate sensitivity is indeed temperature dependent.

3.3. Dislocation analysis of pillars tested at 206 K

To elucidate the rate-controlling deformation mechanism underlying the previously reported mechanical response, the morphology and character of dislocations active during low-temperature plastic deformation were examined. In particular, a detailed TEM analysis was conducted on a micro-pillar deformed at 206 K under a strain rate of 10^{-2} s^{-1} (Fig. 8a, Pillar 12, with corresponding stress–strain response in Fig. 3a), up to a strain level of 2% (Fig. 8). The TEM foil, extracted parallel to the slip trace identified on the pillar surface, is shown in Fig. 8b. The crystal direction normal to the TEM foil was found to be closely aligned with the $[101]$ zone axis. A lattice parameter a of 0.33 nm was experimentally measured for the selected alloy composition based on analysis of the diffraction pattern. We note that no diffuse scattering or distinct diffuse bands connecting the BCC reflections, commonly associated with chemical short-range ordering [86,87], were observed in the diffraction patterns acquired from the material investigated here. Yet, atomic-scale deviations from perfect randomness below the experimental detection limit cannot be excluded.

Dislocation characterization was carried out by tilting the sample to two-beam conditions for three distinct $\mathbf{g}$ -vectors accessible from the $[1\bar{1}1]$ zone axis, specifically, 110 , 011 , and $\bar{1}01$ (Fig. 8c). Two regions of the foil were investigated, namely A and B as indicated in Fig. 8b. Two-beam HAADF images acquired in STEM mode are reported in Fig. 8d and 8e for region A and in Fig. 8f, 8g and 8h for region B. The contrast behavior for each diffraction condition was evaluated against the dislocation invisibility criterion (Table 5) to determine the most likely Burgers vectors. This analysis revealed two distinct dislocation populations with Burgers vectors of $\frac{1}{2}[\bar{1}11]$ and $\frac{1}{2}[11\bar{1}]$, indicated in red and purple in Fig. 8, respectively, both located within the (101) plane (see Fig. 8c).

Beyond the Burgers vector characterization, TEM analysis unveils distinctive dislocation morphologies (Fig. 9). In particular, the microstructure is predominantly characterized by the presence of extended near-screw dislocations (Fig. 9a), which frequently exhibit pronounced tortuosity along their line direction (Fig. 9b), suggestive of localized variations in dislocation line energy associated with the complex chemical landscape or interactions with microstructural obstacles⁽⁸⁾. Across the entire foil, dislocation segments often display

⁷ For the $10^{-3} - 10^{-2} \text{ s}^{-1}$ jump, the mean $\Delta\tau_{\text{CRSS}}$ increments in Table 4 yield $V_{\text{app}}^* = 11, 30.4$, and 46.8 b^3 at 206, 232, and 300 K, respectively, in essentially exact agreement with the values of 11, 30.5, and 46.8 b^3 obtained from the independent constant-rate experiments (Fig. 7a and Table 7).

⁸ The projected line direction observed in the TEM images is considered a close approximation of the true dislocation line direction. Indeed, deformation was observed to occur exclusively on the (101) slip plane, with no evidence of activity on other planes of the same family. The observed dislocations extend across the full width of the pillar and are confined to this well-defined slip plane. Furthermore, the foil normal is within $\sim 1.5^\circ$ of the $[101]$ zone axis, indicating that the specimen surface is nearly parallel to the active slip plane. These geometric constraints significantly limit possible line inclinations and minimize projection effects.

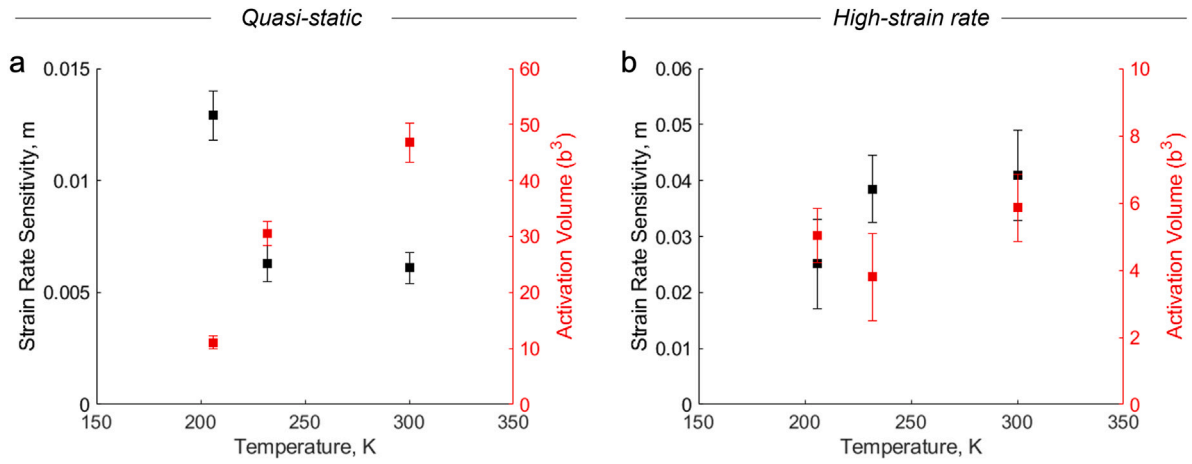


Fig. 7. Temperature dependence of the activation parameters (strain rate sensitivity m and apparent activation volume V_{app}^*) extracted from (a) quasi-static and (b) high-strain rate experiments.

Table 4

Stress increments associated with quasi-static strain rate jumps from 10^{-3} to 10^{-2} s^{-1} at various temperatures and applied strain levels.

T (K)	Strain value (%) at strain rate jump $\Delta\tau_{CRSS}$ (MPa)				Average $\Delta\tau_{CRSS}$ (MPa)
300	7.8% 7.84 ± 2.06	9.8% 8.46 ± 1.31	11.9% 10.57 ± 1.67	14.1% 7.98 ± 2.15	8.72 ± 1.71
232	6.3% 9.07 ± 2.23	8.1% 9.84 ± 1.92	10.2% 11.40 ± 1.35	12.1% 10.40 ± 2.02	10.38 ± 0.98
206	4.9% 24.81 ± 2.55	6.4% 26.9 ± 2.12	8.1% 26.22 ± 2.86	9.7% 23.40 ± 2.52	25.34 ± 2.12

Table 5

Truth table indicating whether $\mathbf{g} \cdot \mathbf{b}$ is non-zero (visible) or zero (invisible) for three distinct $\mathbf{g}$ -vectors accessible from the $[1\bar{1}1]$ zone axis.

$\mathbf{g} \cdot \mathbf{b}$	$\mathbf{a}/2 [111]$	$\mathbf{a}/2 [1\bar{1}\bar{1}]$	$\mathbf{a}/2 [1\bar{1}1]$	$\mathbf{a}/2 [\bar{1}11]$
110	visible	visible	invisible	invisible
011	visible	invisible	invisible	visible
101	invisible	visible	invisible	visible

a distinctive bowed geometry (Fig. 9c,d) indicative of a local character transition from screw to mixed or edge configurations along the dislocation line. This behavior is particularly pronounced in regions approaching the upper surface of the foil (i.e., the micro-pillar boundary) where dislocation lines terminate (see Figure S.4 in the Supplementary Materials).

Interestingly, in a center region of the foil, a full dislocation loop is found, whose geometry reveals a marked anisotropy between the longitudinal and transverse axes, imparting an ellipsoidal character. In Fig. 9e, considering that the Burgers vector $\frac{1}{2}[\bar{1}11]$ is directed from the bottom to the top of the image, the lateral segments of the loop correspond to near-screw character, while the upper and lower arcs are near-edge character. An aspect ratio $A_r = a_2/a_1$ of 0.241 ± 0.028 is measured directly from the traced contour of the loop (Fig. 9f), providing a quantification of the anisotropic nature of the dislocation segment motion, discussed in detail in Section 4.3.

The dislocation density ρ_d was quantitatively assessed from multiple TEM micrographs acquired from different regions across the foil under suitable diffraction conditions. A value of $\rho_{d,2\%} = 3 \times 10^{14} \text{ m}^{-2}$ was measured from the pillar compressed up to 2% of strain. Similar analysis was conducted on a pillar (Pillar 10) subjected to deformation at identical temperature and lower strain rate conditions, compressed up to a strain level of 2.5% (Pillar 10 in Fig. 3a). Corresponding micrographs of the pillar deformed to 2.5% strain, reported in Figure S.4 in the Supplementary Materials, exhibit a similar dislocation morphology as well as dislocation density as for Pillar 12.

3.4. PFDD: Low-temperature critical glide stress measurements and rate analysis

The TEM analysis presented in Figs. 8 and 9 reveals that low-temperature plastic deformation is predominantly governed by the motion of $\frac{1}{2}\langle 111 \rangle$ screw dislocations and their interactions with local solute barriers. These dislocations exhibit characteristic kinked and bowed geometries, indicative of a thermally activated glide process governed by kink-pair nucleation and propagation. The morphological features observed experimentally suggest a strong correlation between dislocation configuration and the rate-controlling mechanism. To quantify this behavior and substantiate the experimental findings, PFDD simulations were employed to evaluate the critical stress to drive the glide of isolated screw dislocations as a function of temperature and strain rate (see “Screw Dipole Configuration” paragraph in Section 2.4).

The simulations span the temperature range 200 K–300 K, providing critical stress values, τ^d , which are normalized by the temperature-dependent isotropic shear modulus $\mu(T)$ (a linear interpolation of the values provided in Table 2 was performed). Simulations were conducted across a range of simulation timesteps corresponding to effective strain rates (see Eq. (4) for the timestep-to-strain rate correspondence).

Results are presented in Fig. 10. The PFDD results quantify the dependence of τ^d on homologous temperature (Fig. 10a) and strain rate (Fig. 10b). The simulations capture the expected trend: decreasing strain rate reduces τ^d , consistent with a thermally activated dislocation glide mechanism.

To further characterize the dislocation mechanism, the strain rate sensitivity, m^d , and activation volume, V^d , were extracted according to:

$$m^d = \left(\frac{\partial \ln \tau^d}{\partial \ln \dot{\epsilon}^d} \right)_{T,\epsilon} \quad (6)$$

$$V^d = \frac{k_B T}{m^d \tau^d} \quad (7)$$

Each dataset was fitted using a power-law function, and m^d values were extracted from the slope of $\ln \tau^d$ vs. $\ln \dot{\epsilon}^d$ plots. The resulting strain rate sensitivities and activation volumes are shown in Fig. 10c. There is strong qualitative agreement between simulations and experiments,

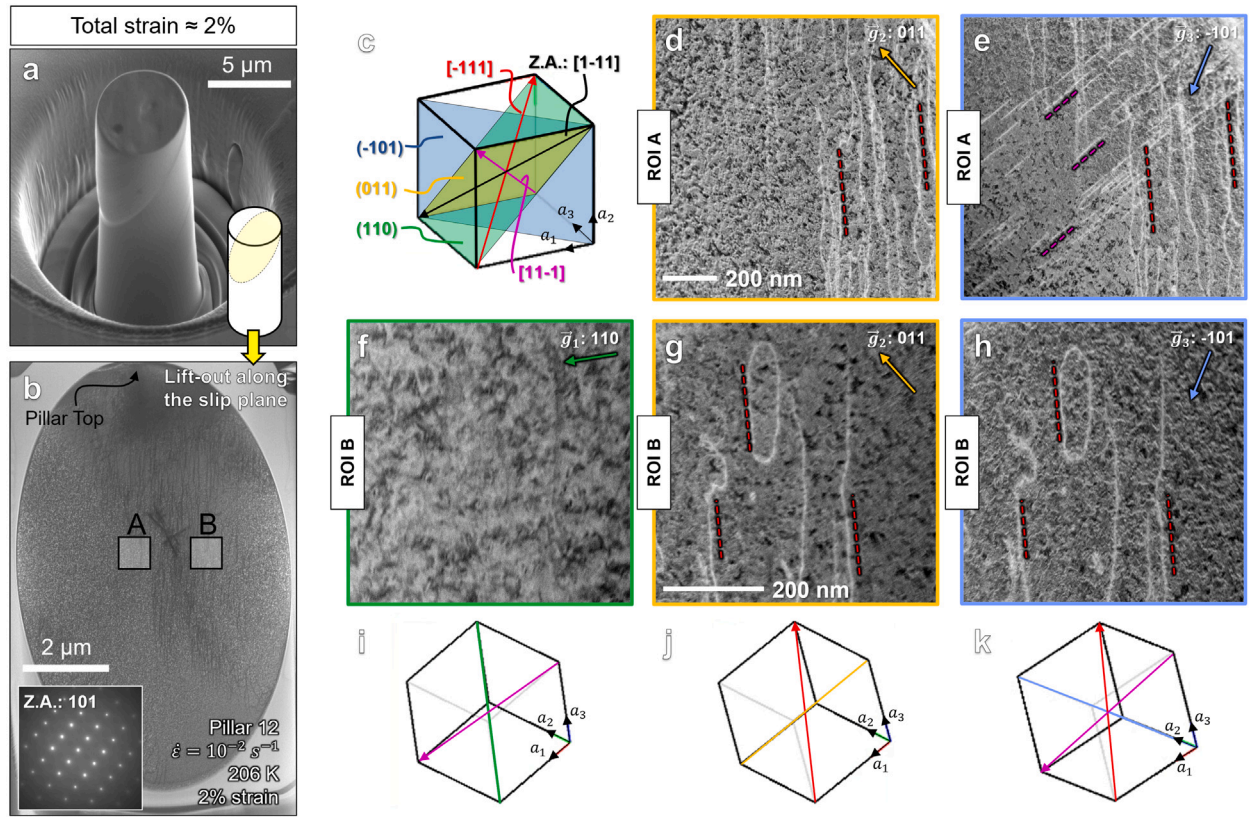


Fig. 8. TEM investigation of a micro-pillar deformed at 206 K and a strain rate of 10^{-2} s^{-1} up to 2% strain. (a) SE image of the deformed pillar (Pillar 12), whose stress-strain response is reported in Fig. 3a, with a τ_{CRSS} of 0.016μ ($\mu = 54 \text{ GPa}$). (b) Bright-field TEM image of the corresponding FIB lift-out lamella, extracted parallel to the surface slip trace. Note that the top region of the foil corresponds to the portion of the pillar surface that was in direct contact with the indenter during deformation. The lamella is oriented with the normal close to the [101] zone axis (see the selective area diffraction pattern (SADP) in inset), consistent with slip on (101) planes. (c) Schematic representation of the diffraction conditions employed to perform Burgers vector analysis using two-beam imaging under three distinct $\mathbf{g}$ -vectors accessible from the [111] zone axis: 110, 011, and $\bar{1}01$. STEM-HAADF images from (d–e) region A and (f–h) region B indicated in (b), highlighting dislocations characterized via invisibility criteria against the selected $\mathbf{g}$ -vectors. Two distinct populations of $\frac{1}{2}[111]$ and $\frac{1}{2}[\bar{1}\bar{1}\bar{1}]$ dislocations are identified and color-coded in red and purple, respectively. The analysis confirms that plastic deformation is mediated by $\frac{1}{2}\langle 111 \rangle$ dislocations, with screw character.

particularly in the temperature dependence of τ^d , as well as in the trends of strain rate sensitivity and activation volume with temperature (Fig. 7a and Fig. 10c). However, the simulated values of τ^d , m^d and V^d are consistently higher, higher and lower, respectively. This discrepancy will be discussed in Sections 4.1 and 4.2. Nonetheless, the trends of the PFDD results corroborate the mechanistic interpretation derived from TEM observations.

4. Discussion

4.1. Analysis of temperature- and strain rate-dependent strength

We first turn to the analysis of the experimentally measured values of the τ_{CRSS} as a function of temperature and strain rate and compare them with theoretical predictions developed for BCC chemically complex alloys. We consider the combined contribution of multiple strengthening mechanisms to τ_{CRSS} in RMPEAs, including intrinsic solid-solution strengthening, τ_{ss} , precipitation strengthening, τ_{p} , grain boundary strengthening, τ_{gb} , dislocation (forest) strengthening, τ_{disl} , and a size-dependent strengthening contribution, τ_{size} . In the present case, EBSD and TEM characterizations confirm a stable single phase (absence of precipitates) in the alloy, while the single crystal micropillar geometry eliminates grain boundary effects. Consequently, τ_{CRSS} can be expressed as

$$\tau_{\text{CRSS}} = \tau_{\text{ss}} + \tau_{\text{disl}} + \tau_{\text{size}} \quad (8)$$

The dislocation strengthening contribution is estimated as $\tau_{\text{disl}} = \alpha \mu b \sqrt{\rho_d}$, where α is taken as 0.5, a typical value for Nb-based systems [88–90], μ is the shear modulus, b is the Burgers vector magnitude, and ρ_d is the dislocation density. Using the dislocation density extracted from Pillar 12 compressed to 2% strain, $\rho_{d,2\%} = 3 \times 10^{14} \text{ m}^{-2}$, τ_{disl} is estimated to be approximately 135 MPa⁽⁹⁾. The size-effect contribution was previously estimated to be on the order of 10 MPa (see Section 3.1). The solid-solution strengthening term τ_{ss} is calculated by employing the Rao–Suzuki (RS) [51] and Maresca–Curtin (MC) [36,37] models. These physics-based analytical models treat τ_{ss} as thermally activated solid solution strengthening, with the RS model attributing the strengthening to solute barriers against screw dislocation glide and the MC model to edge dislocation glide. For completeness, the governing equations and parameters used in these theoretical estimates are reiterated in Section S.5 of the Supplementary Materials. The procedure to determine the solute-screw dislocation interaction energies E_{wi} for the screw mobility RS model is described in Section A.3 of Appendix A. The E_{wi} values for Hf, Mo, Nb, Ta, and Ti solutes in $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$ were determined to be -0.0652 , 0.0897 , 0.0363 , 0.0462 , -0.0652 eV ,

⁹ The absolute dislocation density was not independently measured at each temperature. As a sensitivity analysis, varying ρ_d from 1×10^{14} to $5 \times 10^{14} \text{ m}^{-2}$ changes τ_{disl} from approximately 78 to 174 MPa; because this contribution is added identically to both strengthening models, the relative screw/edge model comparison is unaffected.

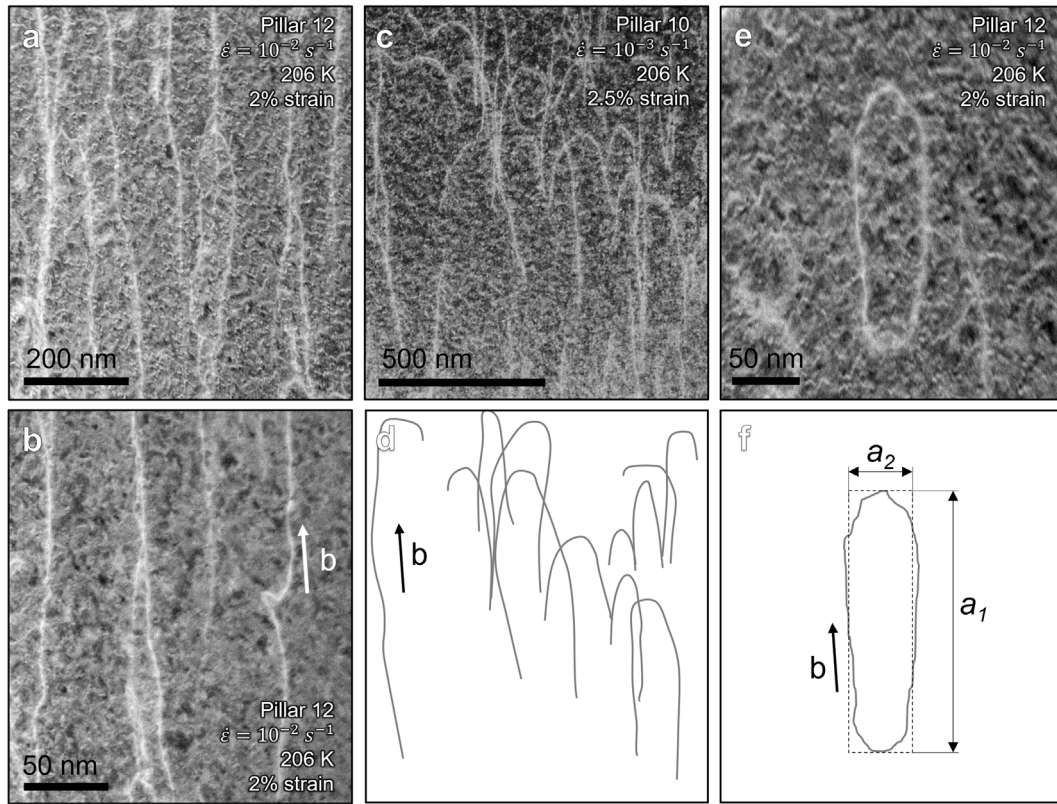


Fig. 9. (a, b) Detailed analysis using STEM-HAADF images of two deformed pillars showing predominantly screw dislocations with kinked morphologies (b). (c) Bowed dislocation segments observed near the top region of the foil, corresponding to the portion of the pillar surface that was in direct contact with the indenter during deformation. The bowed morphology, also schematically represented in (d), indicates local character transition along the dislocation line. A highly anisotropic dislocation loop is observed in the central foil region (e), with a geometry suggestive of differing mobilities for edge and screw components. The traced loop contour (f) confirms its elliptical shape, with an aspect ratio $A_r = a_2/a_1$ of 0.241 ± 0.028 .

Table 6

τ_{CRSS} for $\{110\}\langle 111 \rangle$ slip. Experiments are for the $5 \mu\text{m}$ pillars tested in this work. For τ_{SS} , the second value within the parenthesis corresponds to the contribution of interstitials to strength.

τ in [MPa]	$\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$			$\dot{\epsilon} = 10^{-2} \text{ s}^{-1}$		
	$T = 206 \text{ K}$	232 K	300 K	206 K	232 K	300 K
τ_{CRSS} , experim.	837 ± 18	712 ± 31	616 ± 29	862 ± 19	722 ± 24	625 ± 28
τ_{SS} , screw model	485 (443+42)	456 (415+41)	395 (357+38)	507 (463+44)	478 (436+42)	416 (377+39)
τ_{SS} , edge model	273 (262+11)	265 (254+11)	246 (235+11)	284 (272+12)	277 (265+12)	260 (249+11)
τ_{CRSS} , w/ screw model	630	601	540	652	623	561
τ_{CRSS} , w/ edge model	418	410	391	429	422	405
τ^d , PFDD sim.	–	–	–	1620	1458	1242

respectively. For different T and $\dot{\epsilon}$ conditions, the calculated τ_{SS} values are summarized in Table 6. Note that the alloy contains 0.33 at.% interstitials, and using a generic interstitial solute-screw dislocation interaction energy of 0.5 eV [91]⁽¹⁰⁾, the interstitial contributions to yield at 206, 232 and 300 K are also accounted for and estimated to be 42, 41 and 38 MPa for strain rates of 10^{-3} s^{-1} , and 44, 42, and 39 MPa for 10^{-2} s^{-1} . The contribution of interstitials to strength, added to the edge dislocation model predictions, is also reported in Table 6 and calculated following [47,92] (see also Section S.5.1 in the Supplementary Materials). For different T and $\dot{\epsilon}$ conditions, the predicted τ_{CRSS} values from both the screw and edge dislocation models are therefore obtained by combining the contributions of τ_{SS} , τ_{disl} , and τ_{size} and are reported in Table 6.

¹⁰ Varying the interstitial-screw dislocation interaction energy value from 0.3 to 0.8 eV changes the predicted τ_{CRSS} by only approximately ± 10 MPa on average across all tested conditions.

These model predictions for τ_{CRSS} are compared with experimental data (Fig. 11), where the closest agreement with the experimental data is evident using the RS model. This agreement holds not only for the absolute magnitude of τ_{CRSS} but also for the temperature dependence of the strength, with particularly good correspondence in the intermediate temperature range of 232–300 K. Such agreement suggests that screw dislocations remain the primary strength- and rate-limiting entities controlling plastic deformation in this regime.

While the RS framework provides the closest overall agreement with the experimental data, the MC (edge) model underpredicts the measured τ_{CRSS} by a factor ranging between 1.5 and 2. Although the edge-controlled strengthening description embodied by the MC model does not quantitatively reproduce the measured strength, the stress scales predicted by the edge- and screw-based models remain within a factor of approximately two of one another, representing a substantially smaller separation than typically expected in conventional BCC metals. This comparatively modest separation is also qualitatively consistent with a reduced contrast between edge and screw glide resistance relative to conventional BCC metals. Indeed, the TEM and PFDD

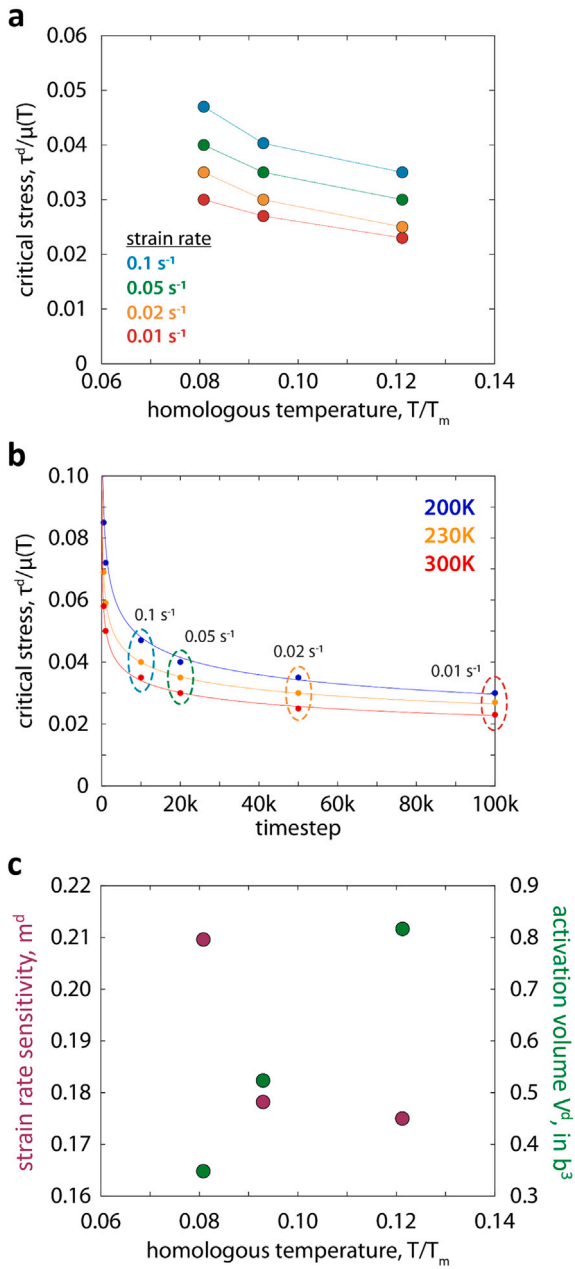


Fig. 10. Temperature and strain rate dependence of the critical stress, τ^d , extracted from PFDD simulations. (a) Normalized $\tau^d/\mu(T)$ as a function of homologous temperature (T/T_m , with $T_m = 2475 \text{ K}$). (b) Effect of strain rate on τ^d , highlighting lower critical stresses at reduced rates, consistent with thermally activated glide. (c) Plot of the strain rate sensitivity m^d and activation volume V^d as a function of temperature. Trends align well with experimental data.

analysis presented in Section 4.3 reveals an effective edge-to-screw mobility ratio of approximately 4 under low-temperature conditions. Thus, although screw segments remain the slower and rate-controlling dislocation character, edge segments are only moderately more mobile and can persist within the deforming dislocation structure rather than rapidly escaping or annihilating.

Consistent with this picture, Section 3.3 shows that near-edge dislocation segments are observed not only near the top of the micropillar, where complex stress states may arise due to indenter–pillar contact and geometric constraints, but also throughout the central region of the pillar (additional TEM micrographs are provided in the Figure S.4 in the

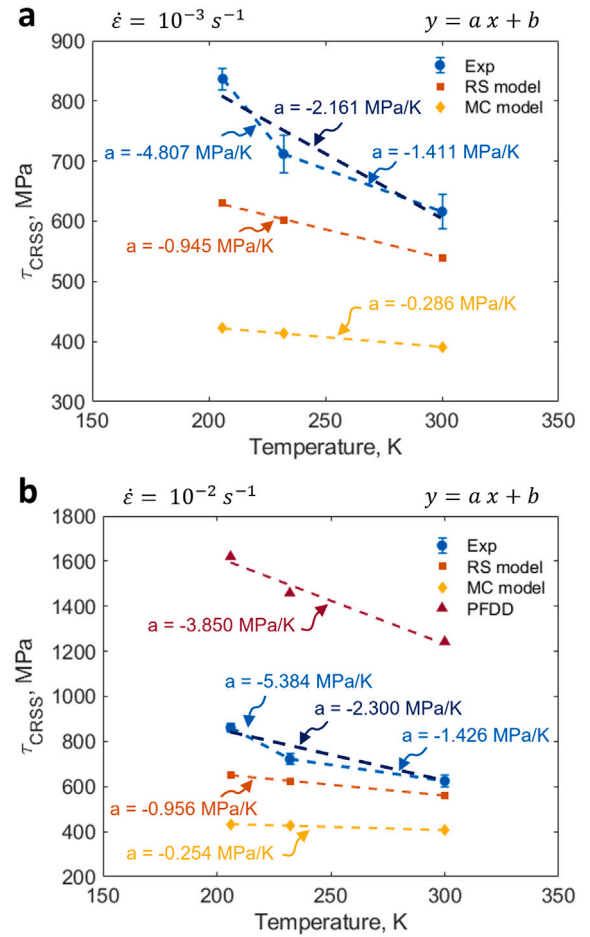


Fig. 11. Temperature dependence of stress: comparison among experiments, simulations, and theoretical models for (a) $\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$ and (b) $\dot{\epsilon} = 10^{-2} \text{ s}^{-1}$. Similar trends can be obtained for $\dot{\epsilon} = 1, 10$ and 100 s^{-1} using the data in Table S.4 and S.5 in Section S.5 of the Supplementary Materials, assuming the same contribution of τ_{disl} and τ_{size} to τ_{CRSS} .

Supplementary Materials). Prior work has shown that edge dislocations can nucleate beneath an indenter and be retained during deformation in RMPEAs [45]; however, the widespread presence of edge dislocation segments well away from the contact-affected zone observed here indicates that reduced edge mobility is an intrinsic feature of the alloy rather than a purely geometric or contact-driven effect. Their retention cannot be attributed solely to localized stress heterogeneities introduced during deformation, but instead reflects an intrinsically reduced edge dislocation mobility, most plausibly arising from heterogeneous energy barriers that stabilize edge segments and suppress their rapid glide and annihilation. This behavior is fundamentally different from conventional BCC dilute alloys, in which edge dislocation segments are notoriously difficult to capture even during *in situ* or postmortem in experimental observations due to their high mobility and rapid escape from the observation volume [31–34].

Taken together, although the edge-based model does not achieve quantitative agreement with the experimental measurements, the microstructural evidence explains why its predictions are closer to the observed strength than would be anticipated from classical BCC behavior. Nevertheless, screw dislocations remain the rate-limiting entities in this alloy across the investigated temperature and strain-rate regime. Despite the mechanistic insight afforded by the RS and MC frameworks, it is evident that neither model reproduces the experimental response across temperature and strain-rate with the level of quantitative accuracy achieved by established strengthening models for pure

BCC refractory metals, such as Johnson–Cook or mechanical threshold stress (MTS) formulations. Further refinement of dislocation-based analytical frameworks, informed by direct experimental validation of operative glide mechanisms, is therefore required to achieve robust predictive capability across composition, temperature, and strain-rate space. In sum, the remaining differences between the RS and MC predictions and experiment may have two possible origins. First, the analytical models necessarily idealize the chemically and mechanically heterogeneous dislocation environment; for example, weak local chemical correlations or nanoscale obstacles below the present experimental detection limit may contribute additional resistance to dislocation glide. Second, even when the rate-limiting dislocation character is correctly identified, the specific elementary glide mechanism assumed by an analytical framework may differ from that operative in the alloy. In particular, the RS model assumes dipole dragging as the rate-limiting low-temperature screw-glide mechanism, whereas the PFDD simulations reveal more complex, temperature-dependent kink-mediated screw-glide processes, as discussed in Section 4.2. Thus, the remaining quantitative discrepancy may reflect both unresolved contributions to the local glide resistance and limitations associated with the specific dislocation mechanism assumed by the analytical description.

We also briefly comment on the origin of the systematic difference observed between the critical glide stresses obtained from PFDD simulations τ^d and the experimentally measured τ_{CRSS} . PFDD consistently predicts higher critical stresses, by approximately a factor of two, across the temperature range investigated. The critical glide stress computed for a single screw dislocation should not be expected to quantitatively match τ_{CRSS} measured even in carefully prepared single crystal deformation experiments. In any real crystal, a pre-existing dislocation density is present from processing, and the long-range stress fields of these dislocations mutually screen one another, collectively lowering the stress required to move any individual dislocation below the single-dislocation glide stress. We ascribe the differences in absolute values of strength and activation parameters between experiment and single-dislocation simulations to the important distinction between collective behavior of long dislocation segments and ensembles (experimental conditions) and individual glide resistance of shorter single dislocation segments (simulations). Furthermore, the higher τ_{CRSS} in PFDD simulations can also result from the finite dislocation line-length effect inherent to the simulations. In this work, PFDD calculations are performed on screw dislocation segments of length $L = 128 b$, corresponding to approximately 37 nm. While our simulated dislocation length is sufficient to allow kink-pair formation, it may still be affected by finite-size effects. Prior work on other RMPEAs has shown a dependence of the critical stress on dislocation line length, with longer dislocations exhibiting lower critical stresses up to a characteristic saturation length [93,94]. Within this context, the observed difference in absolute strength is expected, while the consistent reproduction of temperature-dependent trends of strength and activation parameters reinforces the validity of the underlying physical mechanisms captured by the simulations.

4.2. Analysis of dislocation mechanisms

We next employ PFDD to gain insight into the origins of the experimentally measured activation parameters, which are linked to screw dislocation mobility. Previous PFDD investigations on RMPEAs have shown that screw dislocations exhibit distinct temperature-dependent glide mechanisms [73]. Specifically, it was reported that, independent of applied stress or temperature, spatial variations in the slip plane energy landscape obstruct kink migration to such a degree that the motion of long, initially straight screw segments is not governed by single kink pair (SKP) nucleation and growth [73]. At very low temperatures, screw dislocation motion in RMPEAs rather proceeds via the coordinated nucleation of three or more distinct kink pairs along the line, a process referred to as multiple kink pair (MKP) glide. In this

regime, the screw line remains largely planar, with an average amplitude typically less than $2b$ and predominantly screw character. With increasing temperature, the glide mechanism transitions to overlapping kink pair (OKP) glide, where newly formed kink pairs begin to overlap. This results in segments of the screw protruding $> 2b$ ahead of others and a marked increase in edge- and mixed-character segments along the line. During OKP glide, the dislocation line adopts a wavy morphology but remains largely confined to the habit plane.

To elucidate the underlying glide mechanisms active over the temperature range investigated in this work and relate them to the measured trends in the activation parameters (see Fig. 7a and Fig. 10c), screw dislocation glide mechanisms and mobilities are computed using PFDD for the strain rate $\dot{\epsilon}^d = 0.01 \text{ s}^{-1}$ at $T = 200, 230$, and 300 K . The dominant glide mechanism at each temperature is identified by analyzing line morphology over time. At 200 K (Fig. 12a), MKP glide is the dominant mechanism, while at 230 K (Fig. 12b) and 300 K (Fig. 12c), the glide behavior transitions to OKP glide. In both glide regimes, the underlying energy landscape influences dislocation motion and the associated thermally activated processes. During MKP glide at 200 K , kink pairs preferentially nucleate in low-energy regions, but their migration is hindered by high-energy barriers. To sustain plastic strain under applied stress, additional kink pairs nucleate elsewhere along the line. At 230 K and 300 K , while kinks still become pinned in high-energy regions, the increased thermal energy enables new segments to nucleate atop pinned kinks, allowing the line to search for more favorable pathways through the heterogeneous energy landscape.

Screw dislocation mobility M^d is calculated using the expression $M^d = v/(\tau^d b)$, where v is steady state velocity. Dislocation velocity is determined by linear regression fitting to propagation distance vs. time data. The mobility M^d is found to increase with temperature (Fig. 12d). The increase in mobility between 200 and 230 K is more pronounced than that observed between 230 and 300 K and coincides with the PFDD-resolved transition in the dominant glide mechanism from MKP to OKP glide. Importantly, the experimentally measured and simulated strain rate sensitivity exhibits its largest temperature dependence over the corresponding 206 – 232 K interval (Fig. 7a and Fig. 10c), consistent with the change in glide mechanism identified directly from the PFDD dislocation-line morphologies. At 200 K , the low screw dislocation mobility is accompanied by a high-strain rate sensitivity, consistent with rate-limiting nucleation of multiple kink-pairs occurring in energetically favorable regions. By contrast, the more gradual increase in mobility between 230 and 300 K occurs without a change in the dominant glide mechanism and is therefore associated with a comparatively weaker variation in strain-rate sensitivity over this temperature range.

4.2.1. Activation volumes

We next examine the activation volume, which serves as an effective descriptor of the spatial extent associated with the rate-limiting thermally activated processes governing plastic deformation. At 206 K , the experimentally measured apparent activation volume is $11 \pm 2 b^3$ in the quasi-static regime, indicating a highly localized deformation mechanism. In this regime, plastic flow proceeds through the coordinated nucleation and motion of several kink pairs confined to short segments of the dislocation line, involving only a limited number of atomic spacings and therefore yielding small activation volumes. Interestingly, at 206 K , the experimentally measured apparent activation volume is in good quantitative agreement with the prediction of the RS model (Table 7). The experimentally measured and model-predicted activation volumes are summarized in Table 7, with detailed calculations provided in Section S.5 of the Supplementary Materials.

With increasing temperature, the experimentally measured apparent activation volume increases monotonically, with values in close quantitative agreement with those previously reported for the bulk $\text{Hf}_{15}\text{Nb}_{20}\text{Ta}_{10}\text{Ti}_{30}\text{Zr}_{25}$ high-entropy alloy over the same temperature range [95]. In many crystalline systems, such behavior is commonly

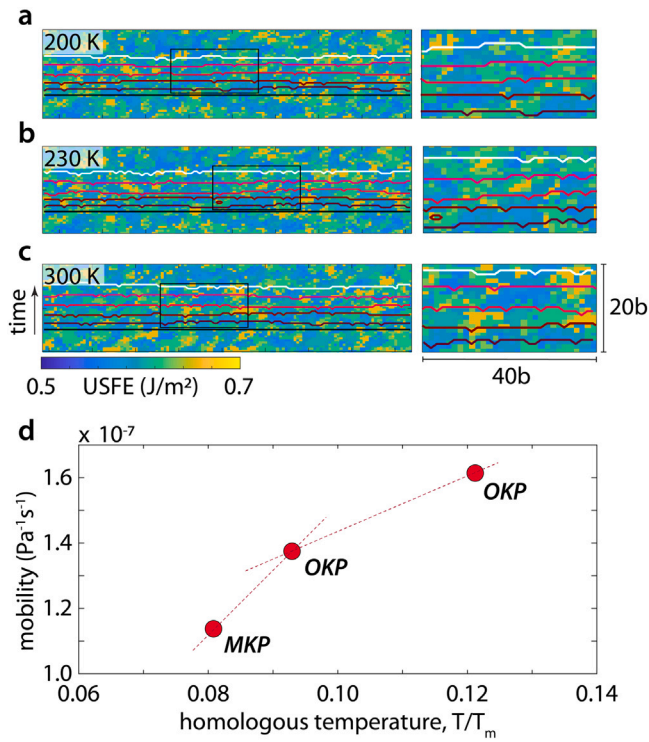


Fig. 12. (a–c) Snapshots of screw dislocation line morphology at six different times, overlaid on the USFE heatmap: (a) 200 K, indicating that MKP glide is the dominant mechanism; (b) 230 K and (c) 300 K, indicating that OKP glide is the dominant mechanism. (d) Screw dislocation mobility M^d as a function of homologous temperature.

Table 7

Activation volume for $\{110\}/\{111\}$ slip.

V^* , in b^3	$\dot{\epsilon} = 10^{-2} \text{ s}^{-1}$		
	206 K	232 K	300 K
V_{app}^* (Experiments)	11 ± 1.2	30.5 ± 2.2	46.8 ± 3.5
$V_{\text{true,screw}}^*$ (RS model)	11	12	16
$V_{\text{true,edge}}^*$ (MC model)	17	18	19
V^d (PFDD sim.)	0.33	0.52	0.83

associated with the activation of additional slip systems or the onset of collective deformation modes involving multiple crystallographic planes. However, in the present RMPEA, plastic deformation remains confined to a single slip system over the entire temperature range investigated. This isolation of single slip activity excludes mechanisms related to slip-system multiplicity or latent hardening and instead points to a temperature-driven evolution of the dislocation glide mechanism with fixed crystallography. The increase in activation volume is therefore also interpreted as a consequence of the transition from MKP-dominated glide at 206 K to OKP glide at higher temperatures. As lattice resistance decreases with increasing thermal energy, screw dislocation motion becomes progressively less localized: kink migration extends over longer portions of the dislocation line, MKP nucleation events become increasingly cooperative, and OKP configurations emerge. These OKP processes involve a substantially larger fraction of the dislocation line and a greater number of participating atoms, naturally giving rise to larger activation volumes. This behavior is particularly significant in the context of RMPEAs as the coexistence of a fixed slip geometry with a strongly temperature-dependent activation volume highlights the capacity of the screw dislocation core to adapt its glide mechanism through changes in collective atomic participation. In this higher-temperature OKP regime, the RS model no longer reproduces the experimentally measured apparent activation volumes. This

discrepancy likely arises from (i) the fundamental difference between the experimentally measured apparent activation volume and the intrinsic true activation volume reported by the model⁽¹¹⁾, and (ii) the inability of the RS framework to capture deformation governed by extended MKP and OKP processes. Consequently, the absolute magnitude of the activation volume is not expected to be accurately described by screw- or edge-based models. The apparent agreement between experiment and RS predictions at 206 K may therefore be fortuitous.

Furthermore, when comparing the experimentally measured apparent activation volumes with those obtained from PFDD simulations, it is immediately evident that the absolute values differ by more than an order of magnitude. In particular, PFDD predicts activation volumes on the order of $\sim 1b^3$, which are significantly smaller than the experimental values (Table 7). Despite this discrepancy in magnitude, the temperature dependence of the experimentally measured apparent activation volume is reproduced more accurately by the PFDD simulations than by either the RS or MC models⁽¹²⁾. The origin of the discrepancy in absolute activation volume values between PFDD simulations and experiments lies in the fundamentally different scales and sensitivities inherent to the two approaches. In PFDD, plasticity is modeled through the motion of a single, isolated screw dislocation, and activation parameters are extracted from the dislocation mobility, defined here through the time required for the dislocation line to advance by a fixed distance. At this scale, the rate-limiting process governing dislocation motion is the lateral migration of individual kink segments, which enables the forward advance of the line by approximately one Burgers vector. This motion of the lateral segment is highly sensitive to the local atomic environment and to discrete energy barriers arising from solute-scale heterogeneity, resulting in a controlling activation volume that is intrinsically small and, indeed, on the order of $1b^3$. With increasing temperature, the formation and migration of OKPs reduces the reliance on the migration of a single pair of lateral kink segments. Nevertheless, even in this regime, the advancement of the dislocation line remains governed by highly localized atomic-scale processes, and the activation volume remains severely small compared to experimental values.

An additional factor contributing to the discrepancy in absolute values is the difference in statistical averaging between experiment and simulation. Experimentally measured apparent activation volumes inherently reflect the collective response of a large population of interacting dislocations. In contrast, PFDD simulations probe the behavior of a single dislocation line evolving within a prescribed energy landscape. As a result, experimental apparent activation volumes represent an effective, ensemble-averaged quantity, whereas PFDD-derived values reflect the activation scale of the elementary rate-controlling process. These differences in scale and averaging naturally lead to discrepancies in the absolute values of activation volume, and similarly in strain-rate sensitivity, between PFDD simulations and experiments. Yet, the ability of PFDD to predict the experimentally observed temperature dependence of the activation volume demonstrates that the simulations capture the correct underlying physical transitions in dislocation glide mechanisms. The agreement in trends, rather than in absolute magnitude, therefore provides strong validation of the mechanistic interpretation derived from PFDD, providing insight on dislocation dynamics that are otherwise inaccessible experimentally.

¹¹ While the apparent activation volume is experimentally determined and may incorporate multiple mechanisms and extrinsic influences, the true activation volume is typically derived from theoretical analyses or atomistic simulations and represents the intrinsic quantity associated with the rate-controlling mechanism.

¹² The temperature dependence is assessed using normalized activation volumes, defined as $[V^*(T)/V^*(200\text{K})] \times 100$, in order to compare relative variations with temperature independently of absolute magnitude. The corresponding rates of change of the normalized activation volume are: (Exp.) 3.182%/K; (PFDD) 1.565%/K; (screw) 0.494%/K; (edge) 0.117%/K.

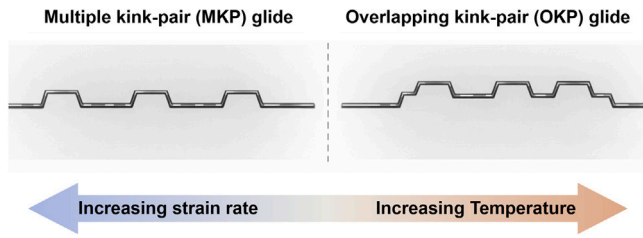


Fig. 13. Schematic illustration of the influence of temperature and strain rate on screw dislocation glide mechanisms.

We next briefly examine the effect of increasing strain rate on the activation parameters. With increasing strain rate, plastic deformation is driven into a regime where higher applied stresses substantially reduce the effective energy barrier for kink-pair nucleation. This stress-assisted activation leads to a reduction in the activation volume. At the highest strain rates investigated, the measured apparent activation volumes approach values on the order of a few b^3 , indicating that highly localized processes, such as repeated individual kink-pair nucleation or the localized bypass of weak obstacles, become rate-limiting. This behavior is analogous to that observed with decreasing temperature. Indeed, at 300 K, an increase in strain rate by five orders of magnitude (from 10^{-3} to 10^2 s $^{-1}$) results in a strength increase comparable to that obtained by reducing the temperature from 300 K to 200 K at constant strain rate (Fig. 5). This correspondence highlights the self-consistency between increasing strain rate and decreasing temperature in thermally activated deformation, as both effectively suppress thermal assistance and shift plastic flow toward more stress-dominated, localized mechanisms (Fig. 13).

4.2.2. Activation energy

Besides the activation volume, the apparent activation energy ΔH_{app} is another relevant thermal activation parameter which provides an effective measure of the enthalpic barrier associated with the rate-controlling thermally activated process governing plastic deformation. The derivation of the apparent activation energy is based on an Arrhenius-type formulation that relates the strain rate $\dot{\epsilon}$ to the applied stress, τ [16,96–98]:

$$\dot{\epsilon} = \dot{\epsilon}_0 \exp \left[-\frac{\Delta H_{app}(\tau)}{k_B T} \right] \quad (9)$$

where $\dot{\epsilon}_0$ is a pre-exponential factor and its dependence on stress and temperature can be neglected and considered constant. Taking the logarithm of both sides yields

$$\log(\dot{\epsilon}) = \log \dot{\epsilon}_0 - \frac{\Delta H_{app}}{k_B T}. \quad (10)$$

Thus, the slope of a plot of $\log(\dot{\epsilon})$ versus $1/T$ provides the value of $-\Delta H_{app}/k_B$. Importantly, this approach assumes that strain rate data compared across different temperatures are evaluated at the same applied stress level, ensuring that variations in strain rate arise solely from thermal activation rather than from differences in stress. In other words, since ΔH_{app} depends on the shear stress τ , ΔH_{app} extracted from the slope of the $\log(\dot{\epsilon})$ versus $1/T$ plot must be associated to an identical stress level for each temperature. To satisfy this condition, experimentally measured strain rate–stress data are interpolated or extrapolated to a common reference stress at each temperature (Figure S.3a in the Supplementary Materials), analogously to the approach used in [99,100]. The strain rates corresponding to this reference stress are then compared across temperatures to extract the apparent activation energy. Figure S.3b in the Supplementary Materials shows the $\log(\dot{\epsilon})$ versus $1/T$ plot constructed using data evaluated at $\tau = 0.74$ GPa. From

the slope of this plot, an apparent activation energy of $\Delta H_{app} = 0.99$ eV is obtained [13].

Physical insight is gained by relating the measured activation energy to the elementary mechanisms of screw dislocation motion. In pure BCC systems, plastic flow at low temperature is governed by kink-pair nucleation along screw dislocations. In RMPEAs, kinks can become locally trapped by variations in the energy landscape, making kink migration, rather than kink pair nucleation alone, a potential rate-controlling process. Atomistic and mesoscale studies of dislocation glide on {110} planes in MoNbTaW [38] reveal that the energy landscape for kink migration is highly rugged, with barriers that vary widely due to local chemical fluctuations. Kinks can become locally trapped, at which point kink pair nucleation takes over to resume dislocation motion (with an overall mean energy barrier of 0.6–0.7 eV). Rather than a clean separation of energy scales, kink migration and kink-pair nucleation actively compete as rate-controlling processes. The apparent activation energy measured here is therefore fully consistent with a regime in which the nucleation and migration of multiple kink-pairs governs the rate-limiting step for screw dislocation glide.

4.3. Loop expansion as a quantitative probe of dislocation segment mobility

We next examine the mobility contrast between screw and edge dislocation segments in the RMPEA. For this purpose, we exploit the geometry of a glissile dislocation loop observed within the TEM foil (Fig. 9e,f). Before considering this loop feature as a yardstick for segment mobility, we first comment on its origin. In RMPEAs, debris loops are most commonly associated with localized cross-slip events, whereby a portion of a dislocation line cross-slips out of its primary habit plane while adjacent segments continue to glide and bow out. As deformation proceeds, the advancing bowed segments may intersect and annihilate, leaving behind a closed sessile loop [38,101,102]. Although debris loop formation is generally infrequent at low homologous temperatures, the spatially heterogeneous energy landscape inherent to RMPEAs enhances the likelihood of localized cross-slip and non-planar dislocation excursions. In the present study, however, aside from this isolated observation, dislocation (and debris) loops are largely absent, consistent with the dominance of single-slip plasticity. By contrast, when multiple slip systems are activated, as demonstrated in the micropillar study on MoNbTi by Balbus et al. [52], extensive cross-kinking interactions lead to a markedly high density of sessile debris loops. Given the single-slip conditions observed throughout deformation in this work, the formation of the present loop is therefore unlikely to originate from cross-kinking interactions.

Another potential mechanism for loop formation could involve the temporary pinning of a localized segment of the dislocation line within a low-energy region of the rugged energy landscape, while neighboring segments remain mobile and continue to glide. As these adjacent segments bow around the pinned region, a closed loop may be left behind in the wake of dislocation motion. Notably, PFDD simulations of glide on the (110) plane (see inset in Fig. 12b) predict the formation of a debris loop trailing a gliding screw dislocation, lending potential support to this interpretation. However, under the thermomechanical conditions relevant to the present experiments, such a pinning-and-bowing mechanism would result in a loop subjected to an inward-directed Peach–Koehler force, promoting loop shrinkage (see Section S.6.1 of the Supplementary Materials). This behavior is inconsistent with the relatively large size of the observed loop (Fig. 9e), suggesting that this mechanism cannot account for its origin and evolution. Given these considerations, we simply conclude that the observed loop is more plausibly the remnant of a complex dislocation process enabled

¹³ Note that using $\tau = 0.85$ GPa, $\Delta H_{app} = 0.91$ eV. That is, the selection of the stress value τ has little influence on the resulting activation enthalpy, at least for the range of stress measured in this work (Fig. 5).

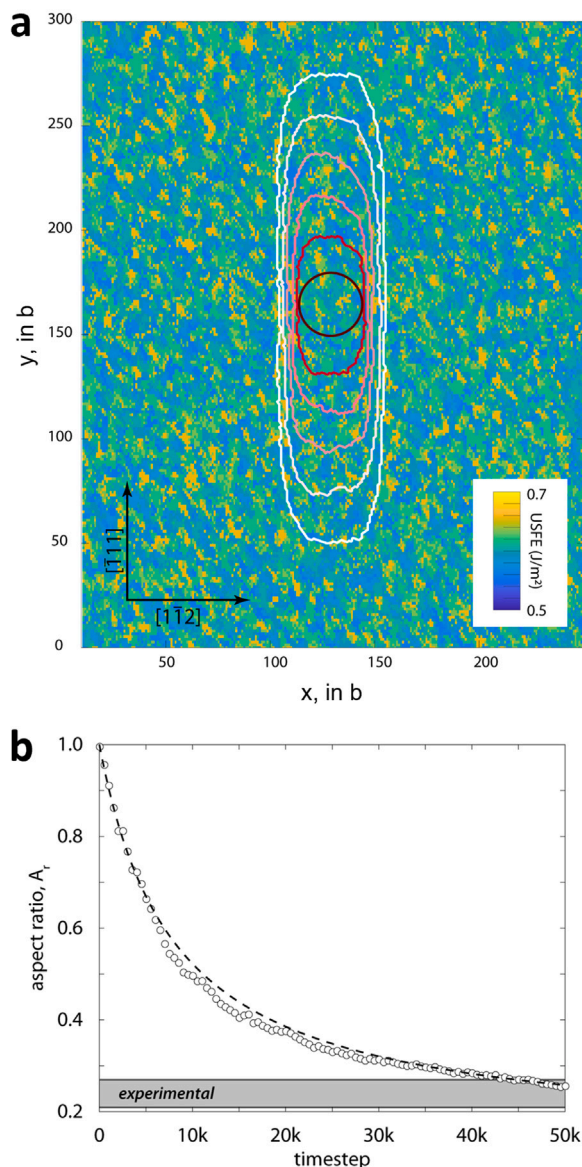


Fig. 14. PFDD simulation of dislocation loop expansion under τ^d at 200 K. (a) Representative example of loop expansion. Dislocation loops are colored with respect to time. Lighter loops indicate a later time step than darker loops. Morphological evolution reveals preferential elongation along directions normal to screw segments, indicating higher edge mobility. (b) Temporal evolution of loop aspect ratio A_r , confirming anisotropic growth kinetics. The simulated aspect ratio bounds encompass the experimentally observed value, providing direct validation of segment-specific dislocation behavior.

by local variations in the solutal stress field. Yet, by the time the loop is observed, the dislocation configuration or source responsible for its formation is no longer present, which precludes a definitive identification of the underlying mechanism.

Once the glissile loop forms, it continues to evolve during micro-pillar deformation, experiencing the same thermomechanical environment as the actively gliding dislocations (see Figure S.7 in Section S.6.2 of the Supplementary Materials for the condition for loop expansion). Note that the loop is located well within the interior of the TEM foil, ruling out contributions from free-surface effects or localized strain fields and reinforcing the fact that it evolves as a direct consequence of the applied stress and temperature conditions. This renders its geometry particularly well suited for quantifying relative dislocation mobility.

Specifically, the upper and lower segments of the loop possess predominantly near-edge character, whereas the lateral segments are of near-screw character. From the measured aspect ratio of the loop, $A_r = 0.241 \pm 0.028$, we estimate that the *effective* mobility of edge segments exceeds that of screw segments by approximately a factor of 4 ($\approx 1/A_r$) at these testing conditions ($T = 200$ K, $\dot{\epsilon} = 0.01$ 1/s)¹⁴.

To quantitatively assess the experimental observations and the preceding discussion against mechanistic predictions, we conducted a series of PFDD simulations tracking the expansion of an isolated dislocation loop under thermally activated glide (see “Dislocation Loop Configuration” paragraph in Section 2.4). In the simulations (Fig. 14a), the expansion dynamics of an initially-isotropic dislocation loop with an initial radius of $16b$ were investigated on the (110) plane at 200 K under an applied shear stress of $\tau^{\text{app}} = \tau^d = 0.03 \mu$, corresponding to a PFDD-effective strain rate of $\dot{\epsilon}^d \approx 0.01$ 1/s (Fig. 10a). These conditions were chosen to closely replicate the experimental thermomechanical environment. By construction, screw segments of the loop lie parallel to the Burgers vector b , while edge segments are oriented perpendicular. As the loop expands under the applied stress, its evolving geometry reflects the relative mobility of these segments and is captured through continuous monitoring of the loop’s aspect ratio $A_r(t)$ (Fig. 14b), defined as the ratio of semi-minor to semi-major axes.

The simulated loop morphology over time exhibits pronounced anisotropy, with the loop elongating preferentially along directions perpendicular to the screw segments, an unambiguous indication that edge segments possess higher mobility than their screw counterparts. As a result, the aspect ratio decays monotonically from unity at $t = 0$ to approximately 0.259 by $t = 50,000$. Strikingly, the experimentally measured aspect ratio of a dislocation loop imaged via TEM at 206 K under equivalent loading conditions falls within the upper and lower bounds of the simulation prediction, providing direct and quantitative agreement between model and experiment. The ability of the model to predict, using only atomistic inputs, the elliptical loop morphology on temperature, segment orientation, and applied stress, confirms that screw dislocations, due to their lower mobility, remain the primary rate-limiting entities controlling plastic deformation in this regime.

To further probe the robustness of this mobility asymmetry and emulate the experiments, a post-mortem simulation was conducted (Fig. 15). After allowing the loop to expand under critical stress for 50,000 timesteps at 200 K, the external stress was removed and the system temperature was raised to 300 K. The simulation was then continued for an additional 200,000 timesteps under zero load. During this interval, a slight reduction in slipped area ($\sim 1.4\%$) was observed, yet the aspect ratio remained essentially unchanged. This invariance implies that both edge and screw segments relax at comparable rates in the absence of driving stress, and that the anisotropy in loop expansion under load is not an artifact of initial conditions but is intrinsically linked to the segmental glide kinetics.

Taken together, these results provide a compelling convergence between experiment and modeling in the study of dislocation mechanics in RMPEAs. Beyond establishing that edge segments are more mobile than screw segments, the present analysis places the mobility disparity on a quantitative scale: under the low-temperature conditions examined here, the effective edge-to-screw mobility ratio is approximately 4. This comparatively modest contrast differs markedly from the conventional description of dilute BCC metals, in which edge dislocations are generally regarded as vastly more mobile than screw dislocations. The chemically heterogeneous energy landscape of the present RMPEA

¹⁴ Because the loop aspect ratio is governed by mobility anisotropy, line energy anisotropy, and elastic interactions, the relation $1/A_r$ is used to extract an *effective* measure of the edge/screw mobility ratio from loop geometry, as would be done with any visual of a loop. Note that just considering line energy disparity, anisotropic elasticity theory predicts $A_r \sim 0.5$ for equal mobilities [103].

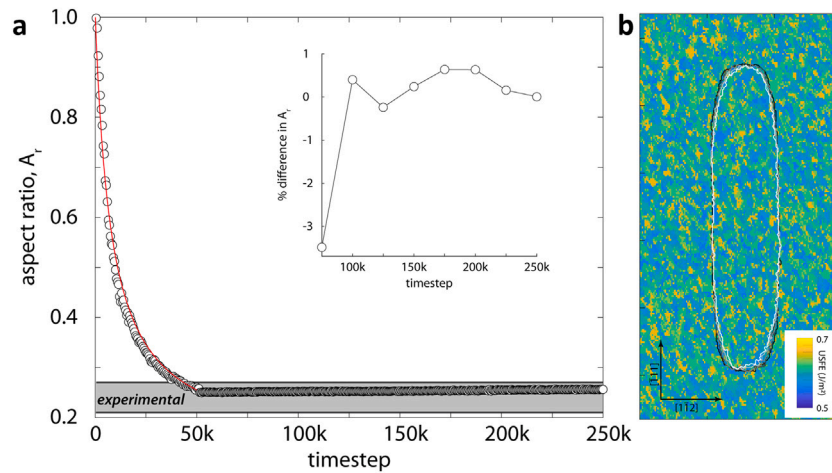


Fig. 15. Post-mortem PFDD simulation showing the evolution of a dislocation loop following unloading at 200 K and annealing at 300 K. (a) Temporal evolution of the loop aspect ratio A_r , with the inset highlighting its percentage change relative to the configuration at unloading (50,000 timesteps). (b) Heatmap of the unstable stacking fault energy (USFE) overlaid with loop morphologies: the black contour corresponds to the loop at unloading (50,000 timesteps), and the white contour shows its relaxed shape (250,000 timesteps).

therefore appears to impose substantial resistance on both dislocation characters, narrowing their mobility separation while preserving screw segments as the slower, rate-controlling entities. This reduced mobility contrast provides a mechanistic basis for the persistent edge segments observed experimentally and indicates that both edge- and screw-character segments can remain dynamically relevant during the evolution of the dislocation structure in chemically complex BCC alloys.

5. Conclusions

This study establishes a mechanistic understanding of the kinetics of single-slip plasticity in the refractory multi-principal element alloy $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$ across 200–300 K and strain rates from 10^{-3} to 10^2 s^{-1} . By combining orientation-controlled micropillar experiments, transmission electron microscopy, analytical modeling, and phase-field dislocation dynamics (PFDD) simulations, a consistent picture of dislocation-mediated deformation emerges:

- **Single-slip isolation:** Exclusive activation of the $\{110\}\langle 111 \rangle$ slip system enabled direct determination of the temperature and strain-rate dependence of the corresponding critical resolved shear stress τ_{CRSS} , free from multi-slip interactions.
- **Dislocation morphology:** TEM reveals extended near-screw dislocations with substantial line tortuosity owing to frequently pinned segments along their line length, together with clearly resolved near-edge segments, reflecting the high lattice friction imposed by the chemically complex energy landscape.
- **Segment-dependent mobility:** A dislocation loop observed within the TEM foil provides a measure of segmental mobility, yielding an effective edge-to-screw mobility ratio of ~ 4 . Remarkably, PFDD simulations independently reproduce this mobility contrast under equivalent thermomechanical conditions. Importantly, this result demonstrates that, although edge segments remain more mobile than screw segments, the disparity is of order a few rather than orders of magnitude. The conventional edge-fast/screw-slow hierarchy of BCC plasticity therefore persists, but is substantially compressed by the chemically heterogeneous energy landscape of the RMPEA.
- **Strength modeling and rate control:** The magnitude and temperature dependence of the τ_{CRSS} are well-captured by the Rao-Suzuki model, confirming screw-dislocation-controlled plasticity and the strength-controlling nature of kink migration. Nevertheless, the edge-controlled description underpredicts the experimental strength by only a factor of approximately 2. Together

with the experimentally determined edge-to-screw mobility ratio, this comparatively modest discrepancy provides independent evidence that edge dislocations experience substantial glide resistance in the RMPEA, even though screw dislocations remain the rate-limiting character over the investigated temperature and strain-rate range.

- **Temperature-dependent activation parameters:** The combined temperature and strain-rate dependence of the τ_{CRSS} yields strain-rate sensitivity, apparent activation volume, and apparent activation energy for $\{110\}\langle 111 \rangle$ slip. These parameters remain strain-independent across the investigated thermomechanical window, indicating that a single governing dislocation mechanism (kink nucleation and migration) controls plastic flow (i.e., dislocation glide) at each temperature condition. An apparent activation energy of $\sim 0.99 \text{ eV}$ measured in this work is fully consistent with a regime in which the nucleation and migration of multiple kink-pairs governs the rate-limiting step for screw dislocation motion.
- **Mechanism transition with temperature:** PFDD simulations qualitatively reproduce the experimentally observed trends in strength, strain rate sensitivity, and activation volume, and are therefore employed to elucidate the temperature-dependent evolution of screw dislocation motion. The simulations reveal a temperature-driven transition in screw dislocation kinetics from a multi-kink-pair regime at 200 K to an overlapping kink-pair regime at 230 K and above. The pronounced change in the experimental activation parameters between 206 and 232 K is consistent with this PFDD-resolved transition. Furthermore, self-consistency between the effects of temperature and strain rate is evident, bolstering the role of thermally-activated deformation processes.

CRedit authorship contribution statement

Nicolò M. della Ventura: Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Julia T. Pürstl:** Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Data curation. **Morgan R. Jones:** Writing – review & editing, Visualization, Software, Methodology, Investigation, Formal analysis, Data curation. **Carolina Frey:** Writing – review & editing, Visualization, Methodology, Investigation, Data curation. **Ravit Silverstein:** Writing – review & editing, Methodology, Investigation, Data curation. **Leah H. Mills:** Writing – review & editing, Visualization, Methodology, Investigation,

Data curation. **Chunhua Tian**: Writing – review & editing, Methodology, Investigation. **Pulkit Garg**: Writing – review & editing, Software, Methodology, Investigation. **Satish Rao**: Writing – review & editing, Software, Methodology, Investigation. **Glenn H. Balbus**: Writing – review & editing, Investigation. **Thomas E.J. Edwards**: Writing – review & editing, Software, Methodology. **W. Streit Cunningham**: Writing – review & editing, Investigation. **Amit Sharma**: Writing – review & editing, Investigation. **Jakob Schwiedrzik**: Writing – review & editing, Resources, Methodology. **Lorenzo Valdevit**: Writing – review & editing, Supervision, Resources, Project administration, Methodology, Funding acquisition. **Xavier Maeder**: Writing – review & editing, Resources, Methodology. **Johann Michler**: Writing – review & editing, Resources, Methodology, Funding acquisition. **Matthew R. Begley**: Writing – review & editing, Supervision, Resources, Project administration, Methodology, Funding acquisition. **Tresa M. Pollock**: Writing – review & editing, Supervision, Resources, Project administration, Methodology, Funding acquisition, Conceptualization. **Irene J. Beyerlein**: Writing – review & editing, Supervision, Resources, Project administration, Methodology, Funding acquisition, Conceptualization. **Daniel S. Gianola**: Writing – review & editing, Supervision, Resources, Project administration, Methodology, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: The co-author Irene J. Beyerlein is an Editor for Acta Materialia and was not involved in the editorial review or the decision to publish this article. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A

A.1. Molecular dynamics simulations of RMPEA energetics

The RMPEA material inputs for the PFDD model were computed through atomistic simulations performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [104]. The atomic interactions in the RMPEA were described using an embedded-atom method (EAM) potential, based on the formulations by Johnson [105] and Zhou et al. [106], specifically developed for the $\text{Hf}_{10}\text{Mo}_{10}\text{Nb}_{35}\text{Ta}_{20}\text{Ti}_{25}$ RMPEA system.

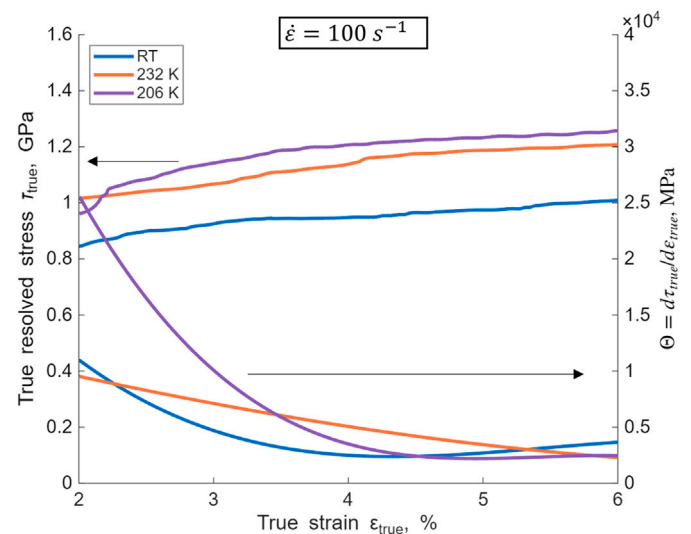


Fig. A.1. True stress–strain curves and corresponding work-hardening rates Θ derived from representative engineering stress–strain data at each test temperature, measured at a nominal strain rate of 100 s^{-1} .

To determine the lattice parameter and bulk elastic constants, a random BCC solid solution supercell containing 2000 atoms and reflecting the desired quinary composition was generated. This supercell was equilibrated using the conjugate gradient algorithm and the Nosé-Hoover thermo/barostat while maintaining periodic boundary conditions in all three spatial directions to extract the equilibrium lattice parameters. The three independent elastic constants, C_{11} , C_{12} , and C_{44} , were obtained by applying the stress–strain method on the equilibrated structure, a well-established approach for calculating elastic properties in crystalline systems [107,108].

For the unstable stacking fault energy (USFE) calculations, a separate random solid solution BCC simulation cell was constructed with the X -axis aligned along the $[111]$ direction (Burgers vector), the Y -axis along the $[110]$ direction (slip plane normal), and the Z -axis along the $[\bar{1}\bar{1}2]$ direction (dislocation line). This USFE simulation cell comprised 35 (110) atomic planes with 48 atoms per plane, totaling 1680 atoms, and measured approximately $2.2 \text{ nm} \times 12.4 \text{ nm} \times 1.6 \text{ nm}$, including a 4 nm vacuum region along the Y direction, with periodic boundary conditions maintained.

The USFE was obtained by rigidly displacing the upper half of the crystal along the slip direction, followed by structural relaxation and energy minimization, allowing atomic relaxation solely in the direction normal to the slip plane [109,110]. While the global composition of the simulation cell matches the experimental composition of the RMPEA, the local composition of each (110) atomic plane differs. Accordingly, the local composition of the stacking fault was defined using two atomic layers along the (110) plane at the shearing interface. To capture the statistical variance of stacking fault energies, multiple shearing layers were sampled along the (110) plane, producing a range of USFE values reflecting the dependence on planar composition.

A.2. Work-hardening rate for $\dot{\epsilon} = 100 \text{ s}^{-1}$

A representative engineering stress–strain curve at each test temperature, obtained at a nominal strain rate of 100 s^{-1} , was transformed into a true stress–strain curve and the corresponding work-hardening rate Θ was computed. The results are illustrated in Fig. A.1. Similar to Fig. 6 for quasi-static loading, the work-hardening rates converge to approximately 4000 MPa above 4% true strain.

A.3. Solute-dislocation interaction energy using MD for $Hf_{10}Mo_{10}Nb_{35}Ta_{20}Ti_{25}$

To calculate solute-dislocation interaction energies for a screw dislocation, a RMPEA simulation cell was constructed and composed by X atoms, i.e. atoms with an average atomic potential. Recent work has shown that, for various functional forms of interatomic potentials, an “average atom” (A-atom) interatomic potential can be rigorously constructed for any random alloy composition [111]. The equilibrium lattice parameter and the 3 elastic constants of the ‘X’ single atom BCC were determined. The simulation cell contained $\sim 200,000$ atoms, with the X-axis aligned along the $[111]$ direction (~ 8 nm), and the Y- and Z-axis oriented along the other orthogonal $[1\bar{1}2]$ and $[1\bar{1}0]$ directions (~ 21 nm). Periodic boundary conditions were applied along the X-axis, while fixed boundary conditions were imposed along the Y and Z directions. The core structure of a $\frac{1}{2}[111]$ screw dislocation was introduced into the RMPEA simulation cell, the system was relaxed and a differential displacement map was made to ensure a compact dislocation core. The first, second, third and fourth nearest neighbors (NN) at the core were identified, following [112]. These selected first, second, third and fourth NN X atoms were substituted with solute atoms to calculate the solute-dislocation interaction energies for the five solute elements, following the methodology described by Rao et al. [42,51,112]. Specifically, for the i th solute constituting the alloy, the solute-dislocation interaction energy at first NN, i.e., E_{1i} was determined by individually substituting the first NN X atom for the solute atom and computing the resulting change in the total energy of the simulation cell. The same substitution was also performed in a defect-free (perfect) lattice to evaluate the corresponding energy change. The interaction energy E_{1i} was thus obtained as the difference between the energy change in the dislocated and perfect configurations with and without solute. Similar procedures were performed to determine the solute-dislocation interaction energies at the second, third and fourth NN, i.e., E_{2i} , E_{3i} , and E_{4i} . The effective interaction energy E_{wi} of the i th solute, was then simply obtained from the following equation [112]: $6E_{4i}^2 + 3(E_{3i} - E_{4i})^2 + (E_{2i} - E_{4i})^2 + (E_{2i} - E_{3i})^2 + (E_{1i} - E_{3i})^2 + (E_{1i} - E_{2i})^2 = 3E_{wi}^2$. The values of interaction energy can be validated by ensuring that $\sum_i c_i E_{wi}$ are equal to (or very close to) zero, with c_i denoting the concentration of solute elements.

Appendix B. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.actamat.2026.122791>.

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