



Full length article

Cryogenic micropillar compression of Ti_3AlC_2 , Ti_3SiC_2 and Cr_2AlC : A comparative evaluation of composition-dependent dislocation mobility in MAX Phases

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ABSTRACT

MAX phases serve as an ideal model system for studying the crossover between metallic and ceramic behavior, and improved ceramic ductility. This ductility is primarily linked to the anomalously easy glide of basal plane dislocations, yet a full theoretical understanding of the characteristics governing their mobility remains a subject of continuing research. Following recent efforts using atomistic simulations of MAX phase basal plane dislocation cores, the present study focused on an experimental evaluation of friction and Peierls stresses in three representative MAX phase compounds, Ti_3AlC_2 , Ti_3SiC_2 , and Cr_2AlC , using micropillar compression at cryogenic temperatures. The study examines specifically the effects of temperature, size, and pristine dislocation morphology under aid of crystal plasticity finite element simulations to derive the lattice resistance for each compound and compare it with previously simulated results. Measured Peierls stresses of 142 MPa (Ti_3AlC_2), 150 MPa (Ti_3SiC_2), and 359 MPa (Cr_2AlC) confirm a significant role of core structures and bonding characteristics on MAX phase dislocation plasticity, with Ti-based MAX phases exhibiting markedly lower lattice resistance than Cr-based compounds. The cryogenic tests presented here mark the first such experiments in MAX phases and open new pathways for understanding their deformation behavior at low temperatures.

1. Introduction

The $\text{M}_{n+1}\text{AX}_n$ phase ternary carbides and nitrides, where M stands for a transition metal, A for an A group element, X for either C or N and $n = 1-4$, have gained widespread interest due to their hybrid ceramic-metallic character [1–3]. Their exceptional properties include high electric and thermal conductivity [1,4–7], high thermal stability as well as pronounced deformability despite limited slip systems [8–14]. The latter is linked to the anomalously easy glide of basal plane

dislocations in the hexagonal crystal [15–18], with experimentally determined critical resolved shear stresses (τ_{CRSS}) at room temperature of as low as 77 MPa [8,19]. While much is known about the electronic structure and functionality of the MAX phases and their 2D derivatives, MXenes [6,20], their basal plane dislocation dynamics remain difficult to resolve. Several concepts regarding dislocation core structures and interactions have been proposed, lately aided by rigorous computational efforts from both density functional theory (DFT) [21,22] and molecular dynamics (MD) [23]. Yet, the exact configurations promoting the observed eased dislocation glide remain under debate.

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MAX phase dislocation mobility is predominantly confined to the metallic layers parallel to the basal plane of the hexagonal crystal [10, 24]. Nevertheless, generalized stacking-fault (GSF) based Peierls-Nabarro models significantly overestimated the resistance to dislocation mobility in the past, with Peierls stresses of ~ 1000 MPa predicted in Ti_2AlN [24] and in Cr_2AlC [25]. This was somewhat reconciled by accounting for the pronounced elastic heterogeneity within the MAX phase crystal [26]. By incorporating individual elasticity parameters from the metallic (M-A) and carbide (M-X) layers determined by DFT, an adapted Peierls-Nabarro framework yielded substantially reduced stress estimates, with for example 26 MPa for Ti_3SiC_2 and 3 MPa for Ti_3AlC_2 [26]. For comparison, experimentally determined critical resolved shear stresses for Ti_3SiC_2 were estimated to 16 MPa using extrapolation from size dependent micropillar compression, and 30 MPa for compression of $10\text{ }\mu\text{m}$ pillars in Ti_3AlC_2 . Whilst the predicted values are in reasonably good agreement with experiments, the exceptionally low Peierls stress estimates, particularly the 3 MPa predicted for Ti_3AlC_2 , raise questions about whether the continuum elastic framework fully captures the resistance to dislocation motion.

Recent reports of non-Schmid effects in MAX phases [11,13] provide experimental evidence that dislocation core structures play a significant role in controlling basal plane dislocation mobility. Plummer et al. [23] and Hossain et al. [21,22] recently used atomistic simulations to investigate different basal plane dislocation core configurations and their Peierls stresses in Ti_3AlC_2 and Ti_3SiC_2 . Using MD, Plummer et al. [23] predicted Peierls stresses of ~ 200 MPa for edge and ~ 3000 MPa for screw dislocations gliding in the M-A layers of Ti_3AlC_2 . The simulations further predicted partial dissociation and the formation of zonal dislocations, a relaxed configuration of a basal dislocation pair, in which two adjacent basal-plane dislocations share the Burgers vector and produce a multi-plane spread core. This paired configuration lowers the local lattice resistance, with Peierls stresses of as low as 20 MPa for edge character. DFT studies by Hossain et al. [21,22] predicted similar Peierls stresses for edge dislocations in Ti_3AlC_2 (~ 200 MPa), as well as ~ 70 – 150 MPa for edge or mixed, and ~ 3000 MPa for screw dislocations in Ti_3SiC_2 . The authors further predicted partial dissociation for both edge and screw characters, yet did not find zonal dislocation formation to be energetically favorable within the DFT framework.

The predicted Peierls stresses for edge dislocations in the above studies are broadly consistent with the range of experimentally measured flow stresses, considering that the atomistic values are obtained under athermal conditions (0 K relaxation and varying effective strain rates). However, experimental evidence of zonal dislocations was so far only provided in Ti_2AlC processed with surface mechanical attrition treatment (SMAT) by transmission electron microscopy (TEM) [27]. Furthermore, no predominance of edge over screw or mixed characters was found during MAX-phase deformation [10,28]. For example, Higashi et al. [10] reported a mix of edge, mixed and screw character after compression of Ti_3SiC_2 , in contrast to the apparent predominance of edge character from simulation.

The predicted predominance of edge character by atomistic simulations suggests either a possible temperature or rate-dependent enhancement of screw dislocation mobility under experimental conditions, or a discrepancy between the predicted core structures and those active in real materials. This motivates further investigation into MAX phase dislocation core structures, as well as temperature dependent deformation. To date, a targeted experimental evaluation of activation parameters or Peierls stresses, which would aid in accurate prediction of dislocation core structures, is outstanding. Such an evaluation can be achieved by probing the temperature-dependence of the τ_{CRSS} , coupled with TEM analysis of dislocation structures. This additionally allows for an estimate of dislocation–dislocation interactions on MAX phase deformation, which is not captured by DFT or MD simulations and may guide further investigations on the basis of dislocation dynamics simulations. So far, experimental evaluation of basal plane dislocation

mobility in MAX phases and the associated τ_{CRSS} has been achieved primarily through compression of textured crystals [8] or via micropillar compression [10,11,13] at room temperature.

The present study incorporates a combined temperature-dependent micropillar compression - TEM protocol to determine Peierls stresses and activation volumes in the Ti_3AlC_2 , Ti_3SiC_2 and Cr_2AlC MAX Phases. This incorporates: (i) a unified micropillar compression methodology to isolate friction stresses based on the study of size effects and crystal plasticity finite element (CPFE) analysis, (ii) testing at cryogenic temperatures (190 K–292 K) to assess thermally activated dislocation glide, and (iii) correlation of mechanical data with targeted TEM to quantify dislocation sub-structures and slip character. The results deliver the first experimentally-determined cryogenic Peierls stresses for MAX phases, activation-volume estimates determined from thermal activation analysis, as well as an initial experimental benchmark to determine the validity of current DFT/MD models of MAX phase dislocation cores. The three model systems selected for the study offer a direct comparison to previous atomistic simulations of dislocation cores, while extending the analysis by variation of the transition-metal chemistry (Ti vs. Cr). The latter is predicted to alter bond hybridization, elastic anisotropy, and hence the intrinsic dislocation core structure. As such, we further use the data to map the plasticity in MAX phases based on bonding characteristics, to actively inform the design of MAX phases or derived systems on the basis of chemistry.

2. Methods

2.1. Materials

Polycrystalline Cr_2AlC ($\sim 99\%$ purity), Ti_3AlC_2 ($\sim 98\%$ purity) and Ti_3SiC_2 ($\sim 95\%$ purity) samples were fabricated via hot isostatic pressing (HIP) of elemental powders for the M and A elements, and either carbon graphite (C) or TiC powders for X in stoichiometric quantities [29,30]. Elemental powder stoichiometry and processing parameters were optimized to minimize the formation of impurity phases, with processing carried out under vacuum to minimize the uptake of impurity elements (O, N, C). The applied processing conditions are summarized in Supplementary Table S.1. To allow for a representative number of pillars to be produced in each selected grain for cryogenic testing, the Ti_3AlC_2 and Ti_3SiC_2 samples were further heat treated at 1300°C for 48 h to induce grain growth, as previously applied by Zhan et al. [11].

Separate specimens were prepared for testing at room and cryogenic temperatures. Samples were cut in the form of semi or quarter disks, and ground to achieve parallel top and bottom surfaces using SiC paper and a 2000 grit fine diamond grinding disk. One surface was further polished using diamond suspensions with progressively smaller particle sizes ($6\text{ }\mu\text{m}$, $1\text{ }\mu\text{m}$, and $0.25\text{ }\mu\text{m}$), followed by a final polish with a H_2O_2 -buffered colloidal silica suspension (OPS, pH 7).

2.2. Orientation analysis

Grain orientations were determined by electron backscatter diffraction (EBSD). EBSD was carried out in a Tescan Lyra 3 with an Oxford Instruments Symmetry Detector (Cr_2AlC , Ti_3SiC_2) and a Tescan Mira 3 fitted with an EDAX EBSD detector (Ti_3AlC_2), using an acceleration voltage of 20 kV, a tilt angle of 70° and a step size of $2\text{ }\mu\text{m}$. Kikuchi patterns were indexed with standard reference cell parameters of $a = 3.073\text{ }\text{\AA}$ and $c = 18.557\text{ }\text{\AA}$ for Ti_3AlC_2 [31], $a = 3.058\text{ }\text{\AA}$ and $c = 17.623\text{ }\text{\AA}$ for Ti_3SiC_2 [32], and $a = 2.86\text{ }\text{\AA}$, $c = 12.82\text{ }\text{\AA}$ for Cr_2AlC [33]. Further orientational analysis was carried out in MTEX [34]. The orientation parameters of selected grains in all three tested compounds are summarized in Supplementary Tables S.2 and S.3.

2.3. Micropillar preparation

Single crystal pillars were prepared by focused ion beam (FIB) milling in distinct grains with high Schmid factors for basal plane slip. Given grain size limitations, and to ensure statistical significance, pillars were prepared in multiple grains for testing at each condition. In addition to a high basal Schmid factor, the grain orientations for milling were chosen such that only one of the three possible basal systems would be favored; geometrically, this corresponds to $\lambda = 90^\circ - \phi$, where λ is the angle between the slip direction and loading axis and ϕ is the angle between the slip plane and loading axis. To further reduce non-Schmid effects [11,13] to a minimum, pillar orientations were selected to maintain Schmid factors for basal plane slip between 0.45–0.5.

Cylindrical pillars with nominal diameters between 1–7 μm and an aspect ratio of 2.5–3 were prepared using annular FIB milling at 30 kV in a Tescan Lyra 3 FIB/SEM and an FEI Helios Nanolab dual beam FIB/SEM. Milling was carried out with gradually reduced milling currents, with a final current of 50 pA for pillars >1 μm in diameter, and 20 pA for pillars 1 μm in diameter, to minimize FIB induced damage and reduce the final pillar taper to below 3° . For temperature dependent testing, a separate set of pillars with a diameter of 3.5 μm was prepared.

2.4. Micropillar compression

Size dependent testing was carried out using an Alemnis nanoinindentation setup (Alemnis Standard Assembly) operated in displacement controlled mode in a Philips XL30 FEGSEM/Tescan Mira 3 SEM. Flat diamond punches, 5 μm in diameter for the 1 μm pillars and 10 μm in diameter for all other pillar sizes (Synton MDP, Switzerland), were used for compression. Compression was carried out at an initial strain rate of 10^{-3} s^{-1} (normalized by pillar height) to a maximum uncorrected strain of 10%.

Temperature dependent testing was carried out using the Alemnis Standard Assembly fitted with a cooling unit for testing at liquid nitrogen temperatures [35] in a ZEISS DSM 962 SEM. Cooling of the cryogenic unit is achieved by a cold finger attached to the back of the indenter, through which gaseous nitrogen is pumped from a liquid nitrogen tank outside the chamber. Sample and tip holders are cooled by connection to the cold finger using copper braids. The cooled region is thermally isolated from the indenter frame by ceramic shafts. Resistive heating and a temperature feedback control loop further minimize variations in frame temperature and frame-related drift.

The measured baseline temperature of the cooling unit were 115 K for the Cr_2AlC and Ti_3AlC_2 test cycles, and 118 K for the Ti_3SiC_2 cycles. To preclude any effects from thermal drift between the sample surface and the flat punch used for compression, each testing cycle at cryogenic temperatures was preceded by thermal equilibration between the tip and sample surface using thermocouples and resistive heaters attached to the tip and sample holders, respectively [36]. Testing was carried out at nominal temperatures of 115/118 K, 200 K and 292 K, corresponding to effective temperatures of $191 \pm 3 \text{ K}$, $233 \pm 3 \text{ K}$ and 292 K. The discrepancy between effective and nominal cryogenic temperatures is linked to thermal losses across the sample thicknesses. The effective surface temperature for each sample was measured in a separate step by approach with a thermocouple fitted to the nanoindenter rig, as described in [36].

Pillars were imaged before and after compression in a Tescan Lyra 3 FIB/SEM. Load–displacement curves were converted to stress–strain data using the pillar height measured for each pillar and pillar-cross section at half the pillar height. In addition to frame compliance, a Sneddon correction [37] was applied to account for pillar sink-in for calculation of strain.

2.5. Transmission electron microscopy

The dislocation structures in the pristine condition material and in pillars post-mortem were further corroborated by means of weak-beam dark field (WBDF) TEM. The pristine dislocation density was evaluated following a line-intersection approach using randomly drawn lines [38,39]. Diffraction contrast analysis ($\mathbf{g} \cdot \mathbf{b}$) was carried out to determine dislocation characters using multiple two-beam conditions corresponding to $\mathbf{g} = \langle 11\bar{2}0 \rangle$ and $\mathbf{g} = \langle 3300 \rangle$ (basal plane reflections). The selected diffraction vectors allow for analysis of full dislocations ($\mathbf{b} = \frac{1}{3}\langle 11\bar{2}0 \rangle$), as well as partial dissociation ($\mathbf{b} = \frac{1}{3}\langle 1100 \rangle$). Details of dislocation density analysis are given in Supplementary Figure S.1 and Supplementary Table S.4; details of diffraction contrast analysis are given in Supplementary Figures S.2–S.7 and Supplementary Tables S.5–S.7.

Lift-outs for TEM analysis were prepared from pristine Ti_3AlC_2 , Ti_3SiC_2 and Cr_2AlC samples, as well as in Ti_3SiC_2 micropillars deformed at room and cryogenic temperatures, using a Tescan Lyra 3 for initial Pt deposition and rough milling and a FEI Helios DualBeam FIB/SEM for fine polishing. Final polishing was carried out at an acceleration voltage of 2 kV and a beam current of 50 pA and a 7° tilt in-plane. Lift-outs of the as produced and deformed samples were prepared with zone axis $[0001]$. TEM analysis was carried out using a ThermoFischer Themis 200 G3 spherical aberration (probe) corrected TEM operated at 200 kV.

2.6. Crystal plasticity simulations

A micropillar crystal plasticity finite element (CPFE) model [40] (Fig. 1(a)) was built in the commercial software package Abaqus to validate the influence of forest hardening on the measured stress–strain responses of the three tested MAX phase compounds, and guide an estimate of friction stresses. The applied mesh reproduced the experimentally measured aspect ratio, with boundary conditions applied to mimic uniaxial compression along the average loading axis determined by EBSD for each compound. Pillar dimensions were normalized with respect to absolute size, to allow for application of a scale-independent constitutive formulation.

The applied constitutive formulation describes a standard finite deformation, anisotropic elasticity as well as a rate-dependent crystal plasticity approach. For the former, the full anisotropic elasticity law with the five independent hexagonal elastic constants corresponding to each MAX phase compound is employed, where:

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix} \begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \epsilon_{23} \\ \epsilon_{13} \\ \epsilon_{12} \end{pmatrix} \quad (1)$$

where $C_{66} = \frac{C_{11}-C_{12}}{2}$ (Fig. 1(b)).

For the later inelastic contribution, deformation is restricted to basal slip mode as the expected predominant deformation mode [10,12,15]. As such, plastic shear was allowed only on the three $\{0001\}\langle 11\bar{2}0 \rangle$ basal slip systems. The resolved shear stress (τ^α) on each active slip system α was related to the shear rate $\dot{\gamma}^\alpha$ by a viscoplastic flow rule, where

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{g^\alpha} \right|^{1/m} \text{sign}(\tau^\alpha) \quad (2)$$

and $\dot{\gamma}_0$ is the reference shear rate, m the strain rate sensitivity exponent and g^α the current critical resolved shear stress on slip system α . The g^α can be further divided into a friction stress (g_0^α) and a hardening component:

$$g^\alpha = g_0^\alpha + \kappa G b \sqrt{\sum_{\beta} \alpha^\alpha \beta \rho^\beta}, \quad (3)$$

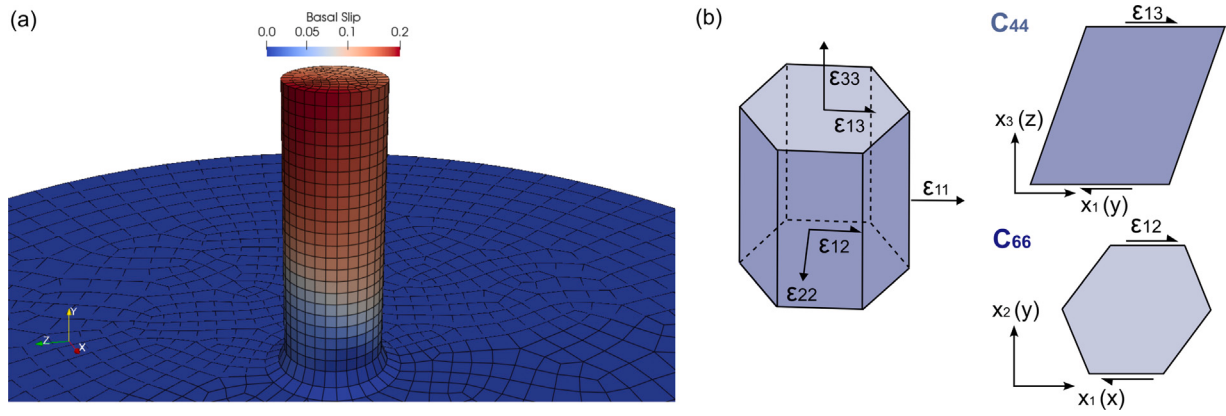


Fig. 1. Outline of CPFE model. (a) Applied pillar mesh (aspect ratio 2.5, no taper) in deformed state, showing activation of a single $\{0001\}\langle 11\bar{2}0 \rangle$ basal slip system. Pillars were oriented to mimic the average orientation for each compound determined by EBSD. Plastic shear is confined to the three $\{0001\}\langle 11\bar{2}0 \rangle$ basal slip systems by setting $g_{0,\text{pyr}/\text{pris}} = 15 \times g_{0,\text{basal}}$ and $\rho_{\text{pyr}/\text{pris}}^{\beta} = 0$. (b) Schematic representation of the five independent elastic constants for hexagonal systems. C_{44} here relates to shear on basal planes (ϵ_{13}); $C_{66} = \frac{C_{11}-C_{12}}{2}$ relates to shear on prismatic planes (ϵ_{12}).

Table 1

Material parameters and interaction coefficients for self and latent hardening for applied CPFE model. Elastic constants from Ref. [43] (Ti_3AlC_2 and Ti_3SiC_2) and Ref. [44] (Cr_2AlC).

Material parameters	b (Å)	C_{11}	C_{33}	C_{44}	C_{12}	C_{13}
Ti_3AlC_2	3.073 [31]	355	293	119	85	76
Ti_3SiC_2	3.058 [32]	370	350	155	97	112
Cr_2AlC	2.863 [33]	396	382	173	117	156
Interaction coefficients	$\alpha^{\text{basal-basal}}$	$\alpha^{\text{prism-prism}}$	$\alpha^{\text{pyr-pyr}}$	$\alpha^{\text{basal-prism}}$	$\alpha^{\text{prism-pyr}}$	$\alpha^{\text{basal-pyr}}$
Ti_3AlC_2	1	1	1	0.5	0.5	0.5
Ti_3SiC_2	1	1	1	0.5	0.5	0.5
Cr_2AlC	1	1	1	0.5	0.5	0.5

where ρ^{β} is the dislocation density on each slip system β with stored forest dislocations, κ and $\alpha^{\alpha\beta}$ are the dislocation interaction coefficient and dislocation interaction matrix for self and latent hardening, respectively, G denotes the effective isotropic shear modulus and b is the Burgers vector. Slip on both pyramidal and prismatic slip systems was here suppressed by assigning an initial critical resolved shear stress $g_{0,\text{pyr}/\text{pris}} = 15 \times g_{0,\text{basal}}$ and fixing their dislocation densities to $\rho^{\beta} = 0$. Within the basal family, one system was treated as mobile (α) and the other two as forest systems (β), each assumed to carry one third of the total initial dislocation density. Eq. (3) accounts for isotropic hardening due to dislocation accumulation. Dislocation-density induced hardening was incorporated by the Kocks–Mecking formulation for dislocation multiplication [41].

The applied material parameters are summarized in Table 1. Interaction coefficients for self ($\alpha^{\alpha\alpha}$) and latent hardening ($\alpha^{\alpha\beta}$) were set to literature-based values for hcp systems [42]. The friction stress τ_0 and dislocation interaction coefficient κ were then varied within expected literature bounds to match bulk critical resolved shear stresses and size-effect corrected initial yield points.

3. Results and analysis

3.1. Pristine microstructure

Scanning electron micrographs of as produced samples are shown in Fig. 2. Both Cr_2AlC and Ti_3SiC_2 show largely equiaxed grains, whilst Ti_3AlC_2 show elongated grains in direction normal to the c -axis. Impurities of predominantly Al_2O_3 , TiC and Cr_7C_3 [29,30] can be seen accumulating along grain boundaries. The grain dimensions

Table 2

Pristine dislocation densities for Ti_3AlC_2 , Ti_3SiC_2 and Cr_2AlC . Pristine dislocations were solely of type $\frac{1}{3}\langle 11\bar{2}0 \rangle$ (Supplementary Figures S.2 - S.7, Supplementary Tables S.5 - S.7).

Compound	ρ_{tot} (m^{-2})	$\mathbf{b}$
Ti_3AlC_2	$1.48 \pm 0.17 \times 10^{14}$	$\frac{1}{3}\langle 11\bar{2}0 \rangle$
Ti_3SiC_2	$3.63 \pm 0.40 \times 10^{13}$	$\frac{1}{3}\langle 11\bar{2}0 \rangle$
Cr_2AlC	$7.84 \pm 0.88 \times 10^{12}$	$\frac{1}{3}\langle 11\bar{2}0 \rangle$

ranged between 5–60 μm in width (w) and 20–180 μm in length (l) for Ti_3AlC_2 , 20–180 μm (l, w) for Ti_3SiC_2 and 10–150 μm (l, w) for Cr_2AlC .

Fig. 2 further shows TEM images of the pristine dislocation structures in the tested MAX phase compounds, imaged along the $[0001]$ zone axis. The observed pristine dislocation network in all three compounds is formed exclusively by $\frac{1}{3}\langle 11\bar{2}0 \rangle$ -type dislocations, as evaluated by $\mathbf{g} \cdot \mathbf{b}$ analysis (Supplementary Figures S.2 - S.7, Supplementary Tables S.5 - S.7). Dislocation densities in each compound are summarized in Table 2. The pristine dislocation densities vary significantly among the three compounds, with Ti_3AlC_2 showing the highest density ($1.48 \times 10^{14} \text{ m}^{-2}$), followed by Ti_3SiC_2 ($3.63 \times 10^{13} \text{ m}^{-2}$) and Cr_2AlC ($7.84 \times 10^{12} \text{ m}^{-2}$). These differences are likely attributed to varying thermal stresses arising during cooling from the synthesis temperature, which scale with the degree of crystallographic anisotropy: the Ti-based compounds exhibit higher c/a ratios (Ti_3SiC_2 : $c/a = 6.04$; Ti_3AlC_2 : $c/a = 5.76$) compared to Cr_2AlC ($c/a = 4.48$). This anisotropy is also reflected in the grain morphology, which evolves from elongated grains in Ti_3AlC_2 to more equiaxed grains in Cr_2AlC (Fig. 2).

The dislocation lines show preferential alignment along the crystallographic $\langle 11\bar{2}0 \rangle$ and $\langle 1\bar{1}00 \rangle$ directions, an observation previously related to elevated lattice friction in Ti_2AlN [28]. The dislocation character observed in Ti_3AlC_2 and Ti_3SiC_2 is solely mixed (30° , 60°) and edge (90°). In Cr_2AlC , short screw (0°) segments are visible in addition to mixed (30° , 60°) and edge (90°) dislocations.

3.2. Micropillar compression

All tested micropillars deformed exclusively by basal slip, with no alternative deformation mechanisms observed at any size, temperature or composition. Representative pillar morphologies and corresponding stress–strain curves are shown in Fig. 3 for room temperature tests (292 K). The curves exhibit characteristic load drops, attributed to discrete yield events such as individual dislocation source activation [12]. Yield stresses were determined as the average of the upper yield stresses

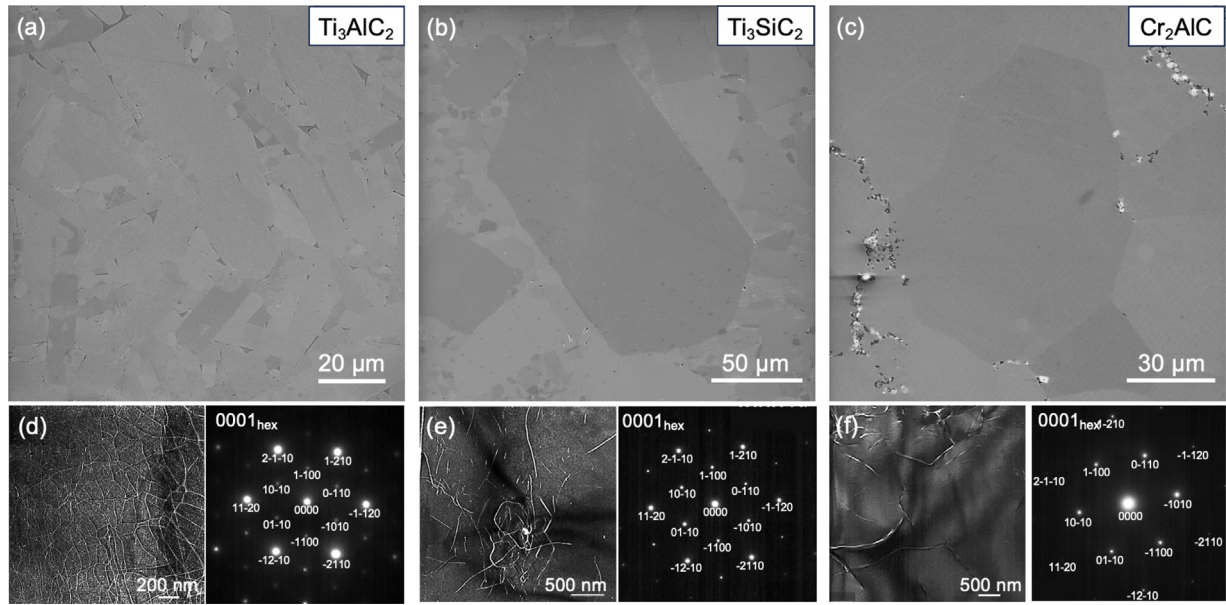


Fig. 2. Pristine microstructure and dislocation network of Ti_3AlC_2 , Ti_3SiC_2 and Cr_2AlC samples. (a) Ti_3AlC_2 shows elongated MAX phase grains ($l = 20\text{--}180\ \mu\text{m}$, $w = 5\text{--}60\ \mu\text{m}$), with few Al_2O_3 globules between grains. A pronounced dislocation network (d) is observed. (b) Ti_3SiC_2 formed MAX phase grains with sizes $l, w = 10\text{--}150\ \mu\text{m}$, with a network of small TiC grains accumulating along grain boundaries. The pristine dislocation network (e) is more localized compared to Ti_3AlC_2 . (c) Cr_2AlC shows equiaxed MAX phase grains with $l, w = 10\text{--}150\ \mu\text{m}$, with Al_2O_3 and Cr_7C_3 accumulating along grain boundaries. The initial dislocation network (f) consisted of few individual dislocation segments.

between 1%–2% plastic strain, in order to avoid artifacts from initial punch alignment [45] and late-stage stress-state breakdown due to pronounced slip activity [12]. To avoid including pillars affected by testing artifacts, data were excluded if the unloading modulus dropped below 70% of the nominal Young's modulus, or if post-compression imaging revealed slip through the pillar top. Such features are likely indicative of bending caused by misaligned loading or the absence of sufficient pre-existing dislocations on the highest-Schmid factor slip systems [45,46].

3.3. Size effects

Fig. 4 summarizes the micro-compression test results aimed at investigating size effects, in the form of τ_{CRSS} as a function of pillar diameter (D) for Ti_3AlC_2 and Ti_3SiC_2 , with results for Cr_2AlC reproduced from a previous study by the authors [13]. The evaluated functional relationships $\tau_{\text{CRSS}} = f(D)$ allow for extrapolation to a bulk critical resolved shear stress, and were further used as a baseline for evaluation of friction and Peierls stresses. For this purpose, an empirical power-law relationship, as commonly used to describe size-dependent strength [45,47–51], was employed to fit the experimental data, with the fit overlaid in Fig. 4. The employed fitting function:

$$\tau_{\text{CRSS}} = \tau_{\text{bulk}} + AD^{-m} \quad (4)$$

describes the experimentally measured τ_{CRSS} by superposition of the bulk critical resolved shear stress, τ_{bulk} , and a size-dependent term determined by material constants A and m , with D as the pillar diameter. τ_{bulk} , A and m were treated as fitting parameters to reproduce the experimental data.

For materials with negligible bulk strength ($\tau_{\text{bulk}} \sim 0$), such as pure metals, the τ_{bulk} term is commonly omitted, reducing Eq. (4) to a two-parameter fit [49]. However, for materials with substantial bulk shear strength, neglecting τ_{bulk} leads to systematic errors in the fitted exponent m and prevents meaningful extrapolation to the bulk limit [50]. Given that MAX phases exhibit comparatively high τ_{bulk} values (e.g., $\sim 70\ \text{MPa}$ for Ti_3SiC_2 [8,19]), the three-parameter formulation was employed here. It should be noted that the inclusion of τ_{bulk} as

a fitting parameter typically results in higher values of m compared to fits that force $\tau_{\text{bulk}} = 0$, as the size-dependent term accounts only for the strength increase beyond the bulk value rather than the total measured strength, resulting in a steeper size dependence. The fitted values of τ_{bulk} and the corresponding extrapolation to the bulk limit are summarized in Fig. 4 for all three tested compounds.

The extracted τ_{bulk} increase in the order $\text{Ti}_3\text{SiC}_2 < \text{Ti}_3\text{AlC}_2 < \text{Cr}_2\text{AlC}$. Based on the pillar deformation morphology, initial dislocation density, and the observed stress–strain response, the mechanisms behind the size dependence are most likely source governed behavior or pre-existing dislocation starvation [52–55].

3.4. Hardening components

The extrapolated τ_{bulk} estimate the stress for basal plane deformation of a macroscopic single crystal. This stress can be further decomposed into a stress from dislocation mobility (i.e., the friction stress at finite temperature) and dislocation entanglement (forest hardening contributions) [45,49,56]. The latter is classically estimated by a Taylor-type hardening component. This is also incorporated in Eq. (3) in the applied CPFPE model, which additionally accounts for dislocation density evolutions during deformation.

The term κ in Eq. (3) is determined by the dislocation interactions within the dislocation forest. In the absence of dedicated dislocation dynamics simulations for MAX phases, these interactions can be estimated from simulations in hcp metals. Bertin et al. [42] estimate $\kappa < 0.2$ for basal-basal interactions in Mg. $\kappa = 0.1$ was hence adopted for the present study.

The simulated loading responses are summarized in Fig. 5. Shown are the calculated τ_{CRSS} as a function of slip evolution, as well as the reference stress strain-curves for Ti_3SiC_2 . The τ_0 denote the intrinsic lattice resistance (Peierls-type friction stress), which was varied until the predicted slip resistance (τ_{CRSS}) matched the experimentally determined τ_{bulk} . This result gives a size-independent calibration, in contrast to fitting directly to size-affected τ_{CRSS} of individual pillars, and is equivalent to decomposing Eq. (3) into friction stress and forest hardening components under consideration of an accumulated dislocation

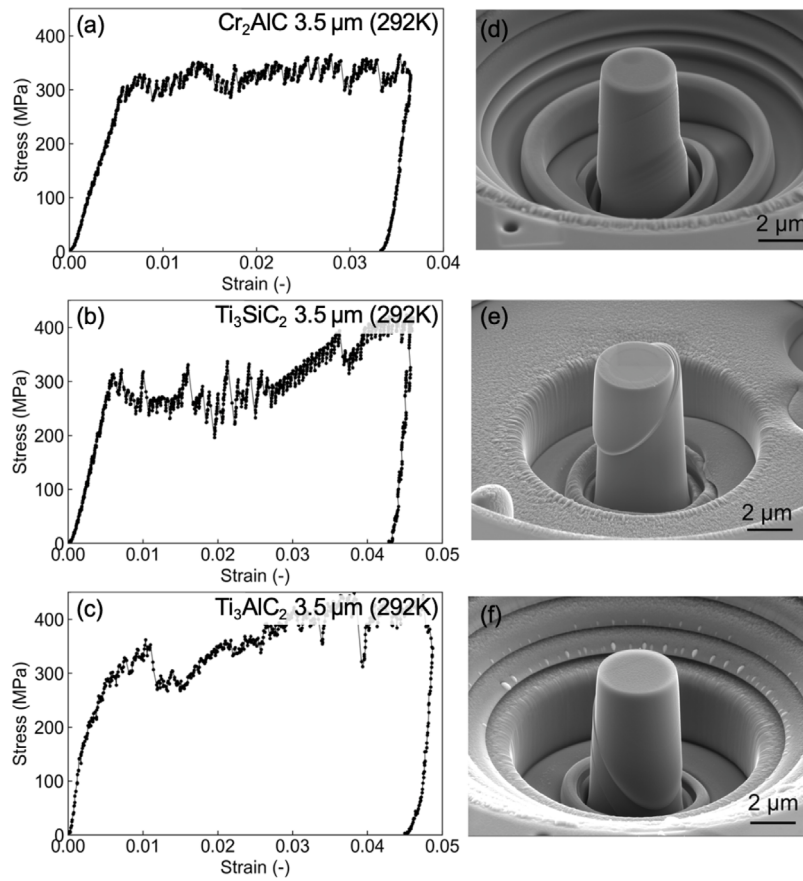


Fig. 3. Loading curves of compressed micropillars (a–c) and associated post-deformation morphologies (d–f) for all three compounds. Pillars deformed solely by basal plane slip. Examples are here shown for a pillar diameter of 3.5 μm , and $T = 292\text{ K}$.

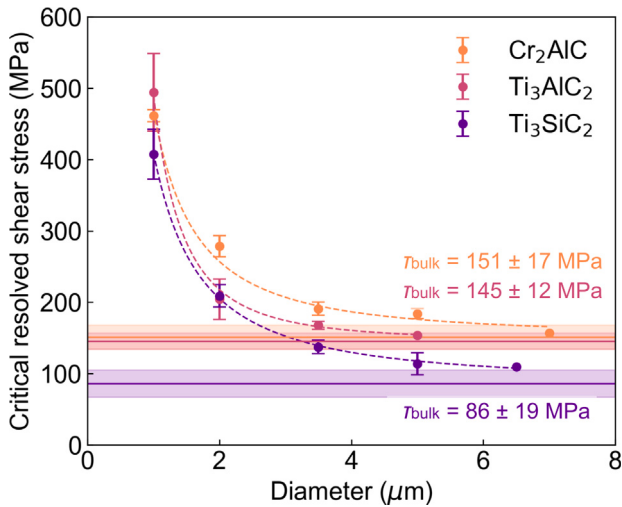


Fig. 4. Size effects determined for Ti_3AlC_2 , Ti_3SiC_2 and Cr_2AlC MAX phase compounds. To assess the τ_{bulk} , the data was fitted to a power law, Eq. (4), using A , m and τ_{bulk} as fitting parameters [13]. Ti_3AlC_2 : $\tau_{\text{bulk}} = 145\text{ MPa}$, $A = 345$, $m = 2.25$; Ti_3SiC_2 : $\tau_{\text{bulk}} = 86\text{ MPa}$, $A = 324$, $m = 1.44$; Cr_2AlC [13]: $\tau_{\text{bulk}} = 151\text{ MPa}$, $A = 317$, $m = 1.58$.

density. The stress–strain curves further confirm that no significant geometric hardening up until 1% strain is present in the deformed pillars, validating the applied methodology for extraction of yield stresses from experimental curves.

Table 3

Results of forest hardening determination in all three compounds. τ_{bulk} signifies the bulk critical resolved shear stress extrapolated from size effect measurements, τ_0 is the friction stress extracted from CPFE pillar models (Fig. 5). A basal dislocation interaction coefficient $\kappa = 0.1$ was used as a primary estimate for all three compounds.

Compound	κ	τ_{bulk} (MPa)	τ_0 (MPa)
Cr_2AlC	0.1	151 ± 17	133 ± 17
Ti_3AlC_2	0.1	145 ± 12	100 ± 12
Ti_3SiC_2	0.1	86 ± 19	65 ± 19

Table 3 lists the determined τ_0 , as well as the τ_{bulk} and adopted κ values. Among the three compounds, Cr_2AlC shows the highest bulk strength, followed by Ti_3AlC_2 and Ti_3SiC_2 . The intrinsic friction stress τ_0 follows the same trend, but reflects differences in initial dislocation density: higher densities increase the Taylor forest hardening component, thus masking the underlying lattice resistance if only the τ_{bulk} is considered. In the present study, this effect is most pronounced for Ti_3AlC_2 . The uncertainties in τ_{bulk} arise from the three-parameter fitting procedure and propagate to the extracted τ_0 values. Uncertainty in the measured dislocation densities ($\pm 10\%$ from TEM analysis) contributes negligibly to the overall uncertainty compared to τ_{bulk} .

3.5. Peierls stress analysis

Friction stress analysis was further extended to cryogenic temperatures to quantify the temperature dependence of slip resistance and to estimate Peierls stresses. Micro-compression tests of pillars 3.5 μm in diameter were performed at effective specimen surface temperatures of $T = 191 \pm 3\text{ K}$, $233 \pm 3\text{ K}$ and 190 K . The results are summarized

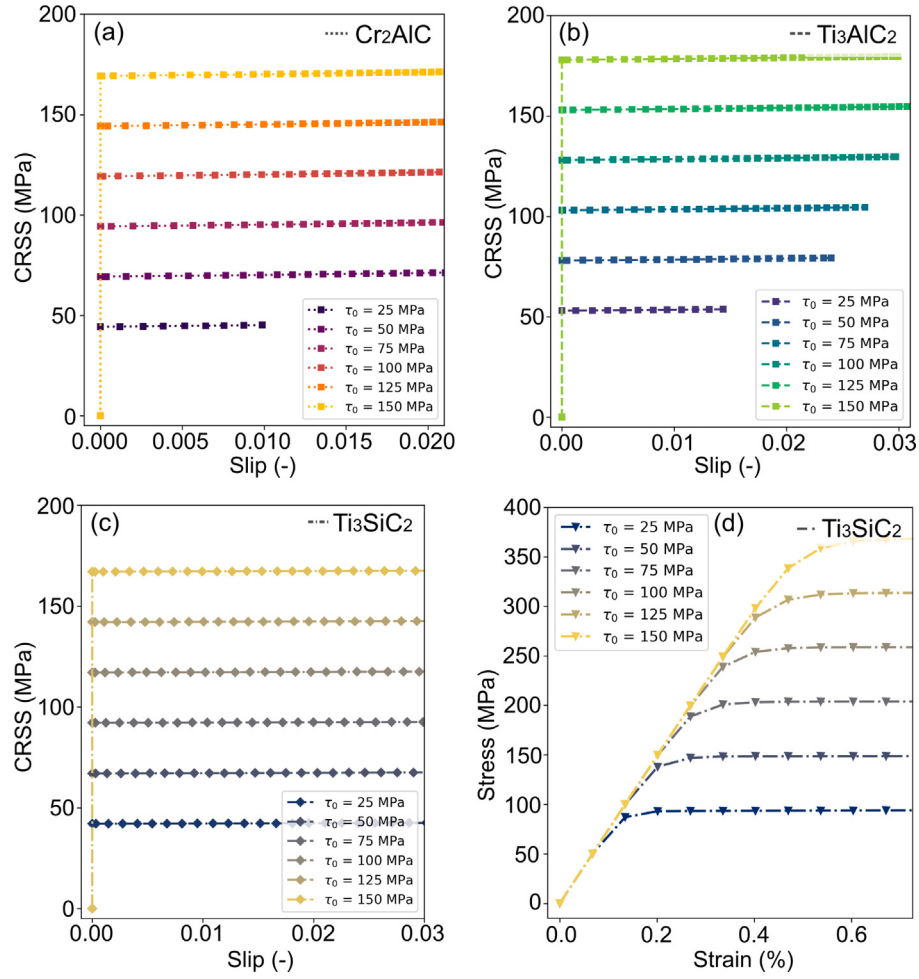


Fig. 5. Forest hardening analysis. (a–c) Critical resolved shear stresses for Cr_2AlC , Ti_3AlC_2 , and Ti_3SiC_2 and (d) associated stress–strain curves for Ti_3SiC_2 determined from CPFE analysis. τ_0 was here determined by matching the size effect corrected τ_{bulk} with the τ_{CRSS} established from CPFE analysis. Cr_2AlC : $\tau_0 = 133$ MPa; Ti_3AlC_2 : $\tau_0 = 100$ MPa; Ti_3SiC_2 : $\tau_0 = 65$ MPa.

in Fig. 6 for all three tested compounds in the form of friction stress versus temperature. Minimal temperature dependency is observed for the Ti-based compounds, with comparably larger temperature dependent behavior for Cr_2AlC . At each temperature, the friction stresses τ_0 were again obtained from measured τ_{CRSS} under consideration of the previously determined size effects (Eq. (4)), and subsequent evaluation of forest hardening contributions from CPFE (Section 3.4). Using the CPFE model, the friction stress $\tau_0^\alpha(T)$ was extracted by first removing the size-dependent contribution from the measured $\tau_{\text{CRSS}}(T)$ according to $\tau_0^\alpha(T) = \tau_{\text{CRSS}}(T) - AD^{-m}$, followed by adjusting $\tau_0^\alpha(T)$ in the CPFE simulations to match this size-corrected bulk strength. Power law coefficients (A , m) and dislocation–dislocation interaction coefficients (κ) were assumed to show negligible temperature dependence over the cryogenic to room temperature range considered, and were thus retained from room-temperature analysis.

Temperature-dependent stress evolution was evaluated using a Boltzmann-type stress-activated process [56,57]:

$$\tau_0 = \frac{kT}{V} \sinh^{-1} \left[\frac{\dot{\gamma}}{2\rho_m v_A b^2} \exp \left(\frac{\tau_p V}{kT} \right) \right], \quad (5a)$$

where k is Boltzmann's constant, V is the activation volume, $\dot{\gamma}$ is the applied shear strain rate, ρ_m is the mobile dislocation density, v_A is the attempt frequency, b is the Burgers vector and τ_p is the Peierls stress. Eq. (5a) can be derived from the Orowan equation:

$$\dot{\gamma} = \rho_m b v, \quad (5b)$$

considering the dislocation velocity, v can be determined from the attempt frequency v_A via

$$v = v_A (P_F - P_B) b, \quad (5c)$$

with P_F and P_B describing the likelihood of a forward or backward jump of a dislocation segment. The probability of a given jump for a stress-activated process is determined by $P_{F/P} = \exp \left[-\frac{V}{kT} (\tau_p \pm \tau_0) \right]$, such that:

$$\begin{aligned} \dot{\gamma} &= \rho_m b^2 v_A \left\{ \exp \left[-\frac{V}{kT} (\tau_p - \tau_0) \right] - \exp \left[-\frac{V}{kT} (\tau_p + \tau_0) \right] \right\} \\ &= \rho_m b^2 v_A \exp \left(-\frac{\tau_p V}{kT} \right) \left[\exp \left(\frac{\tau_0 V}{kT} \right) - \exp \left(-\frac{\tau_0 V}{kT} \right) \right] \\ &= \rho_m b^2 v_A \exp \left(-\frac{\tau_p V}{kT} \right) 2 \sinh \left(\frac{\tau_0 V}{kT} \right), \end{aligned}$$

which can be rearranged to give Eq. (5a).

Eq. (5a) describes the temperature dependence of the lattice resistance (friction stress), rather than that of dislocation–dislocation interaction. The underlying assumption is that dislocation mobility is predominantly governed by the ability of dislocations to overcome the Peierls barrier (lattice resistance), rather than obstacles from impurities or a dislocation forest [46,58–61]. Such an assumption is supported by the observation of straight dislocation segments aligned with distinct crystallographic directions as observed in TEM (Fig. 2) and by the expectation of limited dislocation interactions for basal slip in a basal-plane dislocation network ($\kappa = 0.1$).

Table 4

Input parameters and model identified values for activation volume and Peierls stress following Eq. (5a). $\rho_m = 1/3\rho_{\text{tot}}$; $\nu_A = \frac{k\Theta_D}{h}$. Theoretical τ_p for edge and mixed dislocations determined via MD [23] and DFT [22] were added for comparison.

Compound	$\dot{\gamma}$ (s^{-1})	ρ_m (m^{-2})	Θ_D (K)	ν_A (s^{-1})	V (nm^3)	τ_p (MPa)	$\tau_{p,\text{calc}}$ (MPa)
Ti_3AlC_2	0.002	$4.93 \times 10^{13} \text{ m}^{-2}$	758 [63]	1.58×10^{13}	$1.56 (54b^3)$	142 ± 16	192 [23]
Ti_3SiC_2	0.002	$1.21 \times 10^{13} \text{ m}^{-2}$	780 [63]	1.63×10^{13}	$1.14 (40b^3)$	150 ± 27	70–150 [22]
Cr_2AlC	0.002	$2.61 \times 10^{12} \text{ m}^{-2}$	675 [64]	1.41×10^{13}	$0.37 (16b^3)$	359 ± 63	–

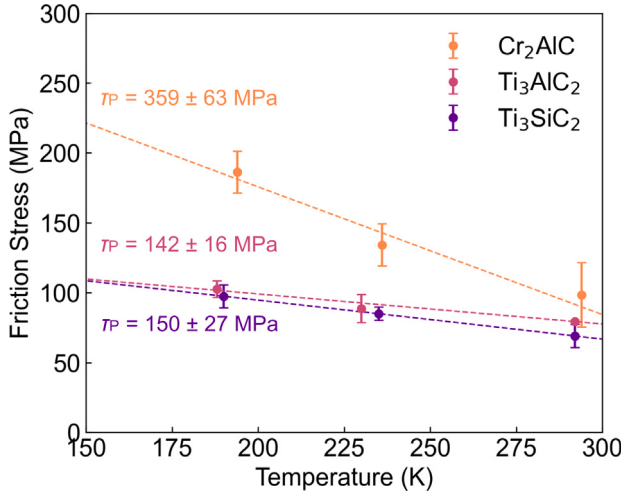


Fig. 6. Temperature dependence of the friction stress measured for Ti_3AlC_2 , Ti_3SiC_2 and Cr_2AlC . The data was fitted to a Boltzmann-type stress-activated process (Eq. (5a)) to assess both τ_p and V . Ti_3AlC_2 : $\tau_0(292 \text{ K}) = 147 \pm 1 \text{ MPa}$, $\tau_0(230 \text{ K}) = 156 \pm 10 \text{ MPa}$, $\tau_0(188 \text{ K}) = 170 \pm 6 \text{ MPa}$, $\tau_p = 142 \text{ MPa}$, $V = 1.56 \text{ nm}^3$; Ti_3SiC_2 : $\tau_0(292 \text{ K}) = 149 \pm 8 \text{ MPa}$, $\tau_0(235 \text{ K}) = 165 \pm 5 \text{ MPa}$, $\tau_0(190 \text{ K}) = 177 \pm 8 \text{ MPa}$, $\tau_p = 150 \text{ MPa}$, $V = 1.14 \text{ nm}^3$; Cr_2AlC : $\tau_0(292 \text{ K}) = 189 \pm 23 \text{ MPa}$, $\tau_0(236 \text{ K}) = 225 \pm 12 \text{ MPa}$, $\tau_0(194 \text{ K}) = 277 \pm 15 \text{ MPa}$, $\tau_p = 359 \text{ MPa}$, $V = 0.37 \text{ nm}^3$.

Estimates of Peierls stresses from temperature dependent friction stress data were obtained by fitting Eq. (5a) to the temperature dependent friction stresses, using τ_p and V as fitting parameters. The resulting fitting curves are overlaid on the experimental data in Fig. 6. All parameters used for fitting are summarized in Table 4, along with the extracted parameters for τ_p and V . The ρ_m were set with $\rho_m = 1/3\rho_{\text{tot}}$, considering slip to occur on one of the three possible basal slip systems. The ν_A can be calculated from Debye temperatures Θ_D via $\nu_A = \frac{k\Theta_D}{h}$ [62]. k and h are the Boltzmann and Planck's constants respectively. The Θ_D in the three compounds were previously determined via ultrasonic sound velocity and heat capacity measurements [63,64].

The highest Peierls stresses were measured in Cr_2AlC ($\tau_p = 359 \pm 63 \text{ MPa}$), which also exhibited the strongest temperature dependence of the friction stress. In contrast, both Ti_3SiC_2 ($\tau_p = 150 \pm 27 \text{ MPa}$) and Ti_3AlC_2 ($\tau_p = 142 \pm 16 \text{ MPa}$) showed lower and comparable Peierls stresses, with a weaker dependence on temperature. The corresponding activation volumes for all three compounds fall within $V = 16 - 54b^3$, consistent with values reported for Peierls-barrier controlled plasticity in hcp or bcc metals [59,60,65], ordered intermetallics [61], or alkali halides [58]. Uncertainties in the extrapolated Peierls stresses reflect both the scatter in temperature-dependent friction stress measurements and the fitting uncertainty in the thermal activation model. Additionally, the absolute magnitudes of τ_p depend on the dislocation interaction coefficient $\kappa = 0.1$ assumed in the CPFEE model. Variation of κ within the range 0.05–0.2 would shift τ_p by ± 20 –35 MPa, but would preserve both the temperature dependence and the relative ranking among compounds, as κ introduces only a systematic offset to the friction stress.

4. Discussion

The primary focus of this study was the experimental evaluation of temperature dependent friction stresses, activation volumes and Peierls stresses in Ti_3AlC_2 , Ti_3SiC_2 and Cr_2AlC , to provide a reference for validating dislocation-core structures predicted by DFT/MD and to determine how chemical variation influences core structure evolution in MAX phases. This was achieved through a combined protocol: evaluation of size effects at room temperature, assessment of forest hardening by crystal plasticity, micropillar compression at cryogenic temperatures, and targeted TEM analysis.

All three compounds showed marked size effects, with predicted bulk critical resolved shear stresses at room temperature of $145 \pm 12 \text{ MPa}$ for Ti_3AlC_2 , $86 \pm 19 \text{ MPa}$ for Ti_3SiC_2 and $151 \pm 17 \text{ MPa}$ for Cr_2AlC . These values are in good agreement with testing of bulk-textured samples [8], where $\tau_{\text{CRSS}} = 77 \text{ MPa}$ for Ti_3SiC_2 [8,19]. The evaluated size effects and forest hardening contributions were further used to extrapolate temperature dependent measurements of τ_{CRSS} to friction stresses, eventually used to determine activation volumes and Peierls stresses.

The results reveal a clear increase in friction stress with decreasing temperature for all three compounds, confirming thermally activated glide. However, the temperature sensitivity ($d\tau_0/dT$) diverges sharply among the compounds, highlighting chemistry-specific Peierls barriers. Cr_2AlC exhibits the steepest increase in friction stresses as a function of temperature, approximately 2.5–3× higher than for the Ti-based MAX phases. Friction stresses in Cr_2AlC rise by $\sim 0.8 \text{ MPa K}^{-1}$ in the quasi-linear region, with Ti_3AlC_2 showing a corresponding rate of $\sim 0.25 \text{ MPa K}^{-1}$, and Ti_3SiC_2 showing a rate of $\sim 0.3 \text{ MPa K}^{-1}$. This predicts the highest Peierls stresses in Cr_2AlC , with $359 \pm 63 \text{ MPa}$, followed by Ti_3SiC_2 with $150 \pm 27 \text{ MPa}$ and Ti_3AlC_2 with $142 \pm 16 \text{ MPa}$.

The experimental Peierls stress predictions for Ti_3AlC_2 and Ti_3SiC_2 are in good agreement with recent DFT calculations and MD simulations of edge dislocation mobility, from which $\tau_p \sim 200 \text{ MPa}$ for Ti_3AlC_2 [21,23] and $\tau_p \sim 70 \text{ MPa}$ for Ti_3SiC_2 [22]. Nevertheless, the Peierls stresses fall below the predicted values for screw dislocations ($\tau_p \sim 3000 \text{ MPa}$) [21–23] and above those suggested for basal dislocation pairs, or zonal dislocations ($\tau_p \sim 20 \text{ MPa}$) [23]. This predominance of edge-type dislocation mobility aligns with the experimental observations from TEM in this work. TEM analysis of pristine Ti_3AlC_2 and Ti_3SiC_2 confirms the sole presence of edge or mixed dislocations; neither pure screw nor zonal dislocations could be detected (Fig. 2, Figure S2 and S6).

To further substantiate the role of edge dislocations in controlling the strength of the Ti-based compounds, TEM analysis was employed post-deformation in Ti_3SiC_2 to highlight the structure and character of operating dislocations. The results are summarized in Fig. 7, Table 5 and further in Supplementary Figures S3–S5 and Supplementary Table S5 for pillars tested at room and cryogenic temperatures. All investigated pillars show evidence of source-governed behavior through $\langle a \rangle$ -type $\frac{1}{3}\langle 11\bar{2}0 \rangle$ dislocation activity. Whilst closely spaced dislocation lines, reminiscent of zonal dislocations with wide dissociation distances [27], are observed, no associated $\frac{1}{3}\langle 1100 \rangle$ type Burgers vectors could be confirmed. The close spacing of dislocations is likely associated with dislocation arrangement (wall formation) in different 0001 planes. The absence of extensive dissociation and zonal dislocations is consistent with DFT predictions of equilibrium core structures

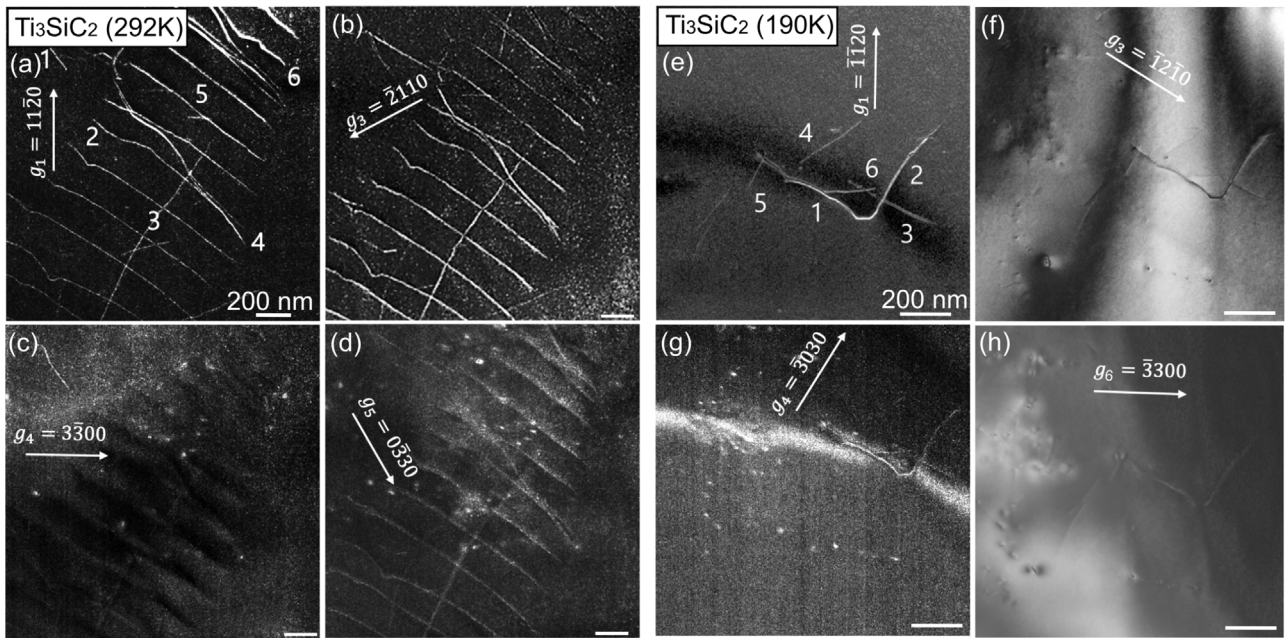


Fig. 7. Post-mortem WBDF TEM analysis at room and cryogenic temperatures in Ti_3SiC_2 ($[0001]$ zone axis). (a–d) 292 K: Parallel dislocation arrays with Burgers vector $\mathbf{b} = \frac{1}{3}[11\bar{2}0]$ observed after room temperature deformation (292 K). (e–h) Isolated dislocation segments (sources) with Burgers vector $\mathbf{b} = \frac{1}{3}[11\bar{2}0]$ observed at cryogenic temperatures (190 K). In both cases, dislocation lines align parallel to $\langle 11\bar{2}0 \rangle$ and $\langle \bar{1}100 \rangle$ directions.

Table 5

Results of $\mathbf{g} \cdot \mathbf{b}$ analysis for Ti_3SiC_2 . Diffraction vectors of type $\mathbf{g} = \langle 11\bar{2}0 \rangle$ and $\mathbf{g} = \langle \bar{1}100 \rangle$ were selected to differentiate between full $\mathbf{b} = \frac{1}{3}[11\bar{2}0]$ and partial $\mathbf{b} = \frac{1}{3}[11\bar{2}0]$ basal dislocation activity.

Deformed (292 K)	$[\bar{1}\bar{1}\bar{2}0]$	$[11\bar{2}0]$	$[\bar{2}110]$	$[\bar{3}030]$	$[03\bar{3}0]$	–	$\mathbf{b}$	Angle between $\mathbf{b}$ & $\mathbf{l}$
1	Y	Y	Y	Y	N	–	$\frac{1}{3}[\bar{2}110]$	90°
2	Y	Y	Y	N	Y	–	$\frac{1}{3}[\bar{1}\bar{1}\bar{2}0]$	60°
3	Y	Y	Y	N	Y	–	$\frac{1}{3}[\bar{1}\bar{1}\bar{2}0]$	30°
4	Y	Y	Y	N	Y	–	$\frac{1}{3}[\bar{1}\bar{1}\bar{2}0]$	60°
5	Y	Y	Y	N	Y	–	$\frac{1}{3}[\bar{1}\bar{1}\bar{2}0]$	60°
6	Y	Y	Y	N	Y	–	$\frac{1}{3}[\bar{1}\bar{1}\bar{2}0]$	60°
Deformed (190 K)	$[\bar{1}\bar{1}\bar{2}0]$	$[11\bar{2}0]$	$[1\bar{2}10]$	$[\bar{3}030]$	$[30\bar{3}0]$	$[\bar{3}300]$	$\mathbf{b}$	Angle between $\mathbf{b}$ & $\mathbf{l}$
1	Y	Y	Y	Y	Y	Y	$\frac{1}{3}[\bar{2}1\bar{1}0]$	60°
2	Y	Y	Y	Y	Y	Y	$\frac{1}{3}[\bar{2}1\bar{1}0]$	30°
3	Y	Y	Y	Y	Y	N	$\frac{1}{3}[\bar{1}\bar{1}\bar{2}0]$	60°
4	Y	Y	Y	Y	Y	N	$\frac{1}{3}[\bar{1}\bar{1}\bar{2}0]$	60°
5	Y	Y	Y	N	N	Y	$\frac{1}{3}[1\bar{2}10]$	90°
6	Y	Y	Y	Y	Y	N	$\frac{1}{3}[\bar{1}\bar{1}\bar{2}0]$	90°

by Hossain et al. [21,22]. As in pristine samples, dislocation lines are preferentially aligned parallel to specific crystallographic directions, highlighting the influence of the lattice resistance on dislocation motion. Contrast analysis again indicates a predominance of edge and mixed (30° and 60°) character.

Further insight into the dominant core characteristics for Ti_3AlC_2 and Ti_3SiC_2 , as well as a first estimate of core structures for Cr_2AlC in the absence of dedicated atomistic simulations, can be obtained from the extracted activation volumes. Specifically, activation volumes of $V_{\text{Ti}_3\text{SiC}_2} = 40b^3$, $V_{\text{Ti}_3\text{AlC}_2} = 54b^3$, and $V_{\text{Cr}_2\text{AlC}} = 16b^3$ were extracted. Peierls-barrier-controlled mobility, for which the dislocation core structure, rather than dislocation–dislocation interactions are the rate-limiting mechanisms in deformation is commonly associated with $V = 1 - 100b^3$ [46,58–61,65]. The observed alignment of dislocation segments with densely packed crystallographic directions supports a pronounced influence of dislocation core structure on mobility. While the comparatively larger activation volumes in Ti_3AlC_2 and Ti_3SiC_2 may link to a transition between a Peierls mechanism and

dislocation-interaction limited mobility, these can be equally explained by a more extended barrier-crossing event, either involving kink-pair formation over longer segments or the cooperative motion of partials. Such dissociation may also be inferred from the post-deformation TEM observations in Ti_3SiC_2 (Fig. 7) in the form of slightly broadened dislocation lines, and is in agreement with the proposed dissociated dislocations in Ti-based MAX phases [10,21–23]. While the presence of zonal dislocations has been proposed previously [27], they were not identified in pristine or deformed samples of any composition in the present study.

Contrary to the Ti-based compounds, the lower activation volume and higher Peierls stress of Cr_2AlC indicate a more localized, thermally activated dislocation motion and correspondingly more compact dislocation cores. Although dedicated atomistic simulations of the dislocation core structures in Cr_2AlC are not yet available, differences between Cr- and Ti-based systems can be further supported by their contrasting non-Schmid sensitivities under uniaxial loading [11,13]. Specifically, Cr_2AlC has been reported to exhibit a decrease in τ_{CRSS}

Table 6

Bond lengths for the p-d hybridized M-A bonds, the correlating M-M and M-X bonds bounding the slip plane, as well as the elastic C_{44} constant in Cr_2AlC , Ti_3AlC_2 and Ti_3SiC_2 .

Compound	M-A (Å)	M-X (Å)	M-M (Å)	C_{44} (GPa)
Cr_2AlC	2.26 [69]	1.98 [69]	2.22 [69]	173 [44]
Ti_3AlC_2	2.88 [72]	2.09 [72]	2.99 [72]	119 [43]
Ti_3SiC_2	2.69 [73]	2.10 [73]	3.05 [74]	155 [43]

with increasing stress normal to the slip plane (σ_n) [13], whereas Ti_3AlC_2 shows the opposite trend, i.e., an increase in τ_{CRSS} with increasing σ_n [11]. A compressive stress normal to the slip plane generally promotes dislocation core widening in plane, thereby lowering the friction stress [66]. This behavior aligns with the observations in Cr_2AlC and supports the presence of initially narrow dislocation cores. In contrast, an increase of τ_{CRSS} with σ_n , as observed in Ti_3AlC_2 , was previously attributed in L_{12} and hcp metals to initially wide dislocation cores that spread across multiple slip planes of different families (e.g., prismatic and pyramidal) [67,68]. Consequently, the pronounced slip-plane inhomogeneity of τ_{CRSS} among these different families likely restricts dislocation mobility under higher σ_n , resulting in the observed increase in τ_{CRSS} . Indeed, dislocation core simulations by MD and DFT support spreading of basal plane dislocations into M-X layers/onto pyramidal planes as an energetically favorable arrangement in Ti-based MAX phases [21,23].

The origin of variations in core structure may be hypothesized to be a consequence of differing bonding characteristics in the examined compounds. Plummer et al. [23] previously suggested A-A bonds as a critical factor related to dislocation core structures based on MD simulations in Ti_3AlC_2 . Yet, the present discrepancies between Cr- and Ti-based MAX phases, and specifically between Cr_2AlC and Ti_3AlC_2 , suggest the M-element to play a more dominant role. Table 6 lists bond lengths for the p-d hybridized M-A bonds, as well as M-X and M-M bonds in the three investigated MAX phase compounds. Overall, Cr_2AlC exhibits shorter bond lengths than both Ti_3SiC_2 and Ti_3AlC_2 , signifying stiffer and stronger bonds in the Cr-based compound [69]. The variation in bond length is mirrored also in the related elastic constants: for example, the C_{44} constant, which relates to shear parallel to the basal plane, is higher for Cr_2AlC compared to the Ti-based MAX phases. Enhanced basal plane slip mobility arises primarily from weaker M-A bonds, in line with GSF considerations [10,24], whereas a confinement of dislocation cores and partial dissociation should be governed additionally by M-M and M-X bonds. Differences in charge density distributions around A atoms, which extend parallel to the M-A layer in Cr_2AlC [69–71], and into the M-X layer in the Ti-based MAX phases [72,73], may additionally contribute to the observed discrepancies in dislocation core structure, although a more detailed bonding analysis is required to clarify this role.

In summary, the measured Peierls stresses and activation volumes for Ti_3AlC_2 and Ti_3SiC_2 are in good agreement with previous predictions of edge and mixed dislocation mobility from MD [23] and DFT [21,22] simulations. TEM analysis of pristine Ti_3AlC_2 and Ti_3SiC_2 , as well as deformed Ti_3SiC_2 samples revealed predominantly edge and mixed ($30^\circ, 60^\circ$) character, with no clear evidence of screw dislocations in the examined samples. This predominance of edge/mixed character and apparent rarity of screw segments suggests that screws are comparably immobile due to their very high Peierls barrier. Screw dislocations are not prominently observed following dislocation generation during thermal stress relief upon cooling from synthesis, nor following active plastic deformation at room temperature and cryogenic conditions, despite their core energies being comparable to those of edge dislocations [23]. In contrast, screw dislocations are clearly present in pristine Cr_2AlC , indicating that screws are sufficiently mobile to be generated and propagate under thermal stresses during cooling. This is consistent with a lower-Peierls screw configuration due to a more compact

dislocation core. Experimentally obtained Peierls stresses and activation volumes confirm more compact dislocation core arrangements for Cr_2AlC , which were effectively linked to stiffer and stronger M-M and M-X bonding characteristics compared to the Ti-based compounds.

While the present experimental findings suggest that dislocation-mediated plasticity in MAX phases is predominantly governed by the Peierls barrier, collective interactions within the dislocation network, in particular with regards to forest hardening, cannot be fully neglected. Future modeling efforts that incorporate atomistic simulations or collective dislocation dynamics in these compounds would provide a valuable addition for determination of the dislocation interaction coefficient κ . Large activation volumes and the less pronounced temperature dependence observed in the Ti-based compounds could further be clarified, particularly regarding the transition between Peierls-dominated and interaction-dominated regimes. The remaining open challenge of resolving dislocation core structures in Cr_2AlC further define a clear target for first-principles modeling.

5. Conclusions

This study presents systematic cryogenic micropillar compression experiments on MAX phases, coupled with size effect analysis, crystal plasticity finite element modeling and TEM characterization to extract both the Peierls stress and activation volumes across three model compounds: Cr_2AlC , Ti_3AlC_2 , and Ti_3SiC_2 . The following conclusions can be drawn:

- Despite their structural similarities, the three MAX phases demonstrated marked differences in Peierls stresses and activation volumes. Cr_2AlC exhibited significantly higher resistance to basal dislocation glide ($\tau_p > 360 \text{ MPa}$, $V \approx 16b^3$), consistent with more compact dislocation cores and stiffer bonding. In contrast, Ti_3SiC_2 and Ti_3AlC_2 showed lower Peierls stresses ($\tau_p \approx 150 \text{ MPa}$) and higher activation volumes ($V \approx 40 - 54b^3$), suggesting more extended core structures and easier shear due to weaker bonding between specifically M-A and M-M atoms. Previously observed differences in non-Schmid effects between Cr_2AlC and Ti_3AlC_2 confirm the likelihood of different core widths in Ti- and Cr-based compounds.
- The determined Peierls stresses in Ti-based MAX phases are in good agreement with DFT and MD predictions for edge and mixed dislocations. TEM analysis of pristine and deformed Ti-based compounds revealed exclusively edge and mixed dislocation character, with no observable screw dislocations. In contrast, screw dislocations were observed in pristine Cr_2AlC , suggesting sufficient mobility to be generated and retained during thermal stress relief upon cooling from synthesis, and consistent with a more compact core structure in this compound. No evidence of zonal dislocations was found in either compound.
- The three MAX phase compounds show marked differences in size effects and pristine dislocation densities. These factors showed a non-negligible influence on forest hardening and apparent strength, masking true friction stress variations between compounds. As such, a comparison with theoretical predictions of dislocation mobility based on chemistry cannot be meaningfully achieved without separating size and forest hardening-related effects from the intrinsic lattice resistance. Future work incorporating dislocation dynamics or larger scale atomistic simulations could help to further elucidate dislocation–dislocation interactions and their influence on plasticity in MAX phases.

CRedit authorship contribution statement

J.T. Pürstl: Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **C. Tian:** Writing – review & editing,

Validation, Methodology, Investigation, Formal analysis, Data curation. **A. Sharma:** Writing – review & editing, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **A. Nascimento:** Writing – review & editing, Visualization, Software, Methodology, Investigation, Formal analysis, Data curation. **N.M. della Ventura:** Writing – review & editing, Investigation, Formal analysis, Data curation, Conceptualization. **T.E.J. Edwards:** Writing – review & editing, Validation, Supervision, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **P. Chartier:** Writing – review & editing, Validation, Resources, Methodology. **M. Vreeswijk:** Writing – review & editing, Validation, Methodology, Investigation. **R.P. Thompson:** Writing – review & editing, Validation, Supervision, Methodology, Conceptualization. **I.J. Beyerlein:** Writing – review & editing, Validation, Supervision, Methodology, Funding acquisition, Formal analysis, Conceptualization. **J.J. Schwiedrzik:** Writing – review & editing, Supervision, Resources, Methodology, Funding acquisition, Data curation. **J. Michler:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Funding acquisition, Conceptualization. **W.J. Clegg:** Supervision, Project administration, Methodology, Conceptualization. **N.G. Jones:** Writing – review & editing, Writing – original draft, Validation, Supervision, Resources, Project administration, Methodology, Funding acquisition, Formal analysis, 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.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.actamat.2026.122432>.

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