

Sintering force underlying the sintering by bulk diffusion

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Abstract

Mass transport by grain boundary diffusion and bulk diffusion leads densification in sintering. Two particles approach driven by the sintering force, the concept of which has been established by analyzing grain boundary diffusion in sintering. A microscopic theory of sintering force is derived for bulk diffusion in this paper. The sintering force for bulk diffusion is defined analogously to that of grain boundary diffusion. It is obtained by replacing the neck curvature by the effective curvature. Numerical simulation of shape evolution is conducted by using the front-tracking boundary element method. The sintering force varied with the contact radius, exhibited a broad peak and became zero at the equilibrium. The simulation results such as sintering force, effective curvature, and relative velocity were presented as functions of contact radius, so that one can predict the dynamics of sintering from the knowledge of particles geometry.

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1. Introduction

Microscopic origin of shrinkage is the center-to-center approach of particles in sintering [1, 2]. The relative velocity of two approaching particles is driven by the sintering force, which can be rigorously defined not only in the sintering of two particles [3-6], but also in the sintering of interacting multiple particles [7-9]. This equation of motion of particles is the basis for the large-scale sintering simulations by the discrete element method (DEM) [10-14]. It is also the key to incorporate the particle motion into the phase-field simulation of sintering; the advection term [15], combined phase-field (PF)/DEM [16], the molecular dynamics-inspired PF simulation [17, 18], phase-field-micromechanics model (PFMMS) [19], and the particle interaction model [20]. The rigid body motion of particles is also included in the Monte-Carlo simulations recently [21, 22]. The sintering forces acting among many particles produces the macroscopic sintering stress, a thermodynamic driving force for shrinkage in the continuum theory of sintering [5, 23, 24]. The observation of particles motion by nanotomography and computer simulation provides new insights into sintering phenomena in multiscale [25].

In sintering of two particles, vacancies formed near the neck surface migrate toward or along the grain boundary either by bulk diffusion or grain boundary diffusion. The mutual movement of particles takes place when vacancies are annihilated at grain boundaries. While both bulk diffusion and grain boundary diffusion contribute to this densifying mechanism, the sintering force has been analyzed only for the case of grain boundary diffusion. The bulk diffusion plays an important role in sintering of relatively coarse particles at relatively high temperatures [26, 27]. For constructing the sintering theory based on micromechanics, it is essentially important to verify whether the sintering force can be defined rigorously for the case of bulk diffusion.

Two atomic diffusion paths are distinguished for bulk diffusion; one from surface to neck surface and the other from grain boundary to surface. The former is the non-densifying mechanism, and the latter is the densifying mechanism. Kuczynski [28] focused on the neck growth in sintering by non-densifying mechanism. Kingery and Berg [1], Coble [2], Johnson and Clarke [29], and Wilson and Shewmon [30] studied the densification by bulk diffusion and expressed the shrinkage as a function of time. Several diffusion paths involve sintering simultaneously; surface diffusion, grain boundary diffusion, and bulk diffusion [27]. Such complicated problems are analyzed by computer simulations; bulk diffusion without rigid body motion [31-34], coupled surface/bulk diffusions [35], coupled grain-boundary/bulk diffusions [36, 37], coupled surface/grain-boundary/bulk diffusions [38] and described in a review [39].

We present here a theory of sintering force in the sintering only by bulk diffusion (volume diffusion or lattice diffusion) for simplicity. For simulating the shape evolution during sintering, we used a front-tracking approach based on the boundary element method solving problems governed by the Laplace equation [40].

2. Modelling

2.1 Force balancing

Consider the sintering of two identical spheres by bulk diffusion as illustrated in Fig. 1. The diffusive flux in the bulk is proportional to the gradient of the diffusion potential $\Phi = \mu_a - \mu_v$, where μ_a and μ_v are chemical potential of atoms and vacancies respectively [41]

$$\mathbf{j} = -\frac{D_B}{kT\Omega} \nabla \Phi \quad (1)$$

D_B is the diffusion coefficient in the bulk, k is the Boltzmann constant, Ω is the atomic volume, and T is the absolute temperature. Mass conservation in the bulk gives

$$\nabla^2 \Phi = 0 \quad (2)$$

We solve the Laplace equation under following boundary conditions. The surface and grain boundary are assumed to be perfect source/sink of vacancies so that the vacancies are maintained in equilibrium; thereby, the chemical potential of vacancy is zero $\mu_v = 0$. The diffusion potential depends on the normal traction σ_n acting on the surface and grain boundaries

$$\Phi = \mu_a = \mu_0 - \sigma_n \Omega \quad (3)$$

where μ_0 is the chemical potential under a flat surface. The normal traction on the free surface S is the product of surface free energy per unit area γ_s and the curvature κ , the sum of two principal curvatures,

$$\sigma_n = \gamma_s \kappa \quad (4)$$

The curvature is defined as negative, $-2/r_0$, for a spherical particle with radius r_0 in this paper. The normal traction on a spherical particle surface is negative and compressive.

In the sintering of two identical particles in Fig. 1, the force acting on a circular contact with radius c is given by surface tension along the surface triple junction. The

integral of normal traction on the contact area $A_c = \pi c^2$ is [3, 9]

$$F_c \equiv \int_{A_c} \sigma_n dA = -\gamma_s L_c \sin(\psi/2) \quad (5)$$

where $L_c = 2\pi c$ is the circumference, and ψ is the dihedral angle. The equilibrium dihedral angle ψ_{eq} is given by the ratio of the grain boundary free energy per unit area γ_{gb} to the surface energy γ_s

$$\gamma_{gb} = 2\gamma_s \cos(\psi_{eq}/2) \quad (6)$$

The force and stress are positive for tension and negative for compression. The contact area is subjected to a compressive force due to the force balance. We assume D_B , γ_s , and γ_{gb} are isotropic and independent of crystal orientation.

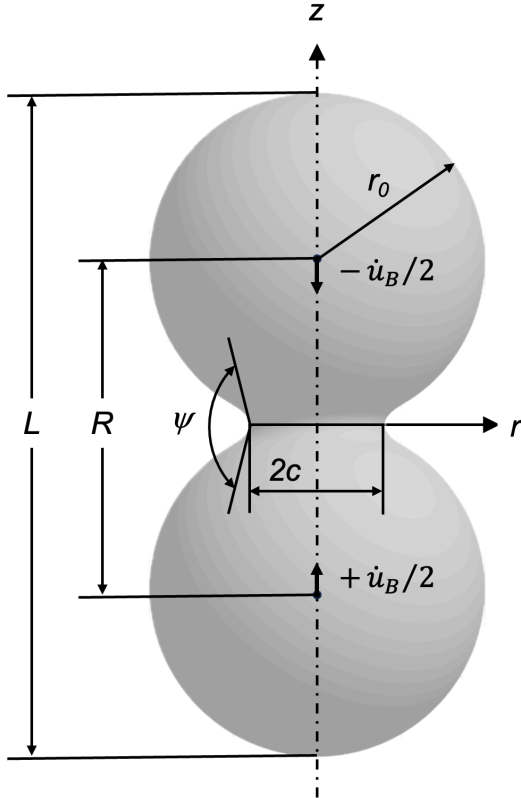


Fig. 1 Sintering of two spherical particles. The black dot inside a particle indicates the mass center. The distance of mass centers, R , and the pair length, L , are defined in the

figure.

2.2 Equation of motion in sintering

When matter is transferred to/from the surface, the normal velocity v_n of the surface is proportional to the flux j_n normal to the surface

$$v_n = j_n \Omega \quad (7)$$

Two particles approach when vacancies are annihilated at grain boundary. The relative velocity of two particles is proportional to the chemical potential gradient at the contact plane A_c ($z = 0$),

$$\dot{u}_B = -\frac{2D_B}{kT} \left(\frac{\partial \Phi}{\partial z} \right)_{z=0} \quad (8)$$

The coefficient is 2 because the vacancy flux comes to contact plane from both sides. As two particles approach by the rigid body motion, $\dot{u}_B$ and $(\partial \Phi / \partial z)_{z=0}$ are constant over the contact plane. The total surface motion is a sum of surface motion by Eq. (7) and the rigid body motion by Eq. (8).

Since the Laplace equation is linear, we can decompose the solution into two subproblems:

$$\Phi - \mu_0 = -(\varphi + q_0 \phi) \Omega \quad (9)$$

Both φ and ϕ are harmonic functions. The function φ and the weight coefficient q_0 have the dimensions of stress, and ϕ is a dimensionless function.

Sub-problem 1 (non-densifying solution): $\nabla^2 \varphi = 0$

Solve the Laplace equation with:

Free surface: Dirichlet $\varphi = \gamma_s \kappa$

Contact plane ($z = 0$): Neumann $\partial \varphi / \partial z = 0$

Sub-problem 2 (densifying solution): $\nabla^2 \phi = 0$

Solve the Laplace equation with:

Free surface: Dirichlet $\phi = 0$

Contact plane ($z = 0$): Neumann $\partial \phi / \partial z = 1/r_0$

Both sub-problems have fully known boundary conditions and are straight forward standard boundary element method (BEM) solves.

Substituting the decomposition, Eq. (9), into the force balance integral constraint, Eq. (5):

$$\int_{A_c} (\varphi + q_0 \phi) dA = F_c$$

Solving for q_0 :

$$q_0 = \frac{F_c - \int_{A_c} \varphi dA}{\int_{A_c} \phi dA} \quad (10)$$

At the contact plane $z = 0$, the Neumann condition of the sub-problem 2 gives

$$\left(\frac{\partial \Phi}{\partial z} \right)_{z=0} = - \frac{q_0 \Omega}{r_0} \quad (11)$$

From Eqs. (8) and (11), the relative velocity is proportional to the weight coefficient q_0

$$\dot{u}_B = \frac{2D_B \Omega}{kT r_0} q_0 \quad (12)$$

From Eq. (10) and (12), the equation of motion is given by

$$\dot{u}_B = - \frac{2D_B \Omega}{kT g^* c^3} F_B^S \quad (13)$$

where F_B^S is the sintering force for bulk diffusion

$$F_B^S = \gamma_s \kappa^* A_c + \gamma_s L_c \sin(\psi/2) \quad (14)$$

κ^* is an effective curvature

$$\gamma_s \kappa^* \equiv \frac{1}{A_c} \int_{A_c} \phi dA \quad (15)$$

Since the integral of ϕ on the contact area scales with c^3 , we introduced a dimensionless geometric factor g^*

$$\int_{A_c} \phi dA \equiv g^* \left(\frac{c}{r_0}\right)^3 r_0^2 \quad (16)$$

3. Numerical simulation by boundary element method

3.1 Boundary element method

The sintering of two identical spherical particles was simulated using an axisymmetric sharp-interface boundary-element method. The calculation was formulated in the meridional $r - z$ plane, and the three-dimensional particle shape was obtained by rotation about the symmetry axis in Fig. 1. Owing to symmetry, only the upper particle was explicitly discretized; the lower particle was represented by reflection with respect to the grain boundary plane $z = 0$. The particle surface and the circular grain boundary contact were represented by piecewise-linear boundary elements.

The diffusion problem was decomposed into two linear sub-problems, sub-problem 1 and sub-problem 2. The boundary integral equation was assembled using the axisymmetric Green's function for Laplace's equation. The kernel was evaluated by numerical quadrature along each boundary element, with complete elliptic integrals used for the azimuthally integrated Green's function. This procedure gives dense boundary-element matrices [40]. A mixed boundary-value problem was solved at each time step: Dirichlet conditions were imposed on free-surface elements and Neumann conditions on grain-boundary elements. The resulting dense linear systems were solved directly.

The simulations were carried out using custom Python codes developed by the authors. During code implementation, ChatGPT (OpenAI) and Claude (Anthropic) were used as auxiliary programming tools for drafting selected code segments, debugging, and improving code structure. The scientific model, numerical procedures, code verification, and interpretation of the simulation results were determined by the authors.

3.2 Motion of surface and triple junction

From Eqs. (1), (7), and (9), the surface normal velocity is given by

$$v_n = \frac{D_B}{kT} \left(\frac{\partial \phi}{\partial n} + q_0 \frac{\partial \phi}{\partial n} \right) \quad (17)$$

The total surface motion in sintering is the sum of the surface normal velocity, Eq. (17), and the rigid body motion, Eq. (13)

$$\mathbf{v} = v_n \mathbf{n} \pm \frac{1}{2} \dot{u}_B \mathbf{e} \quad (18)$$

where $\mathbf{n}$ is the unit normal vector to the surface, and $\mathbf{e}$ is the unit normal vector to the contact plane. The normal velocity, Eq. (17), was applied only to the free-surface shape change. The rigid body translation associated with densification was applied separately as a downward translation of the upper particle with speed $-\dot{u}_B/2$.

Figure 2 illustrates normal velocity and the rigid body motion at the contact point C . The motion of the contact point was treated using a dynamic contact-line condition. The kinetic contribution to the contact radius velocity was written as

$$\dot{c} = \dot{u}_B \cot(\psi/2)/2 + v_n(C) \sin(\psi/2) \quad (19)$$

where $v_n(C)$ is the one-sided limiting value of the free-surface normal velocity at the contact point, approximated by the value on the last free-surface element.

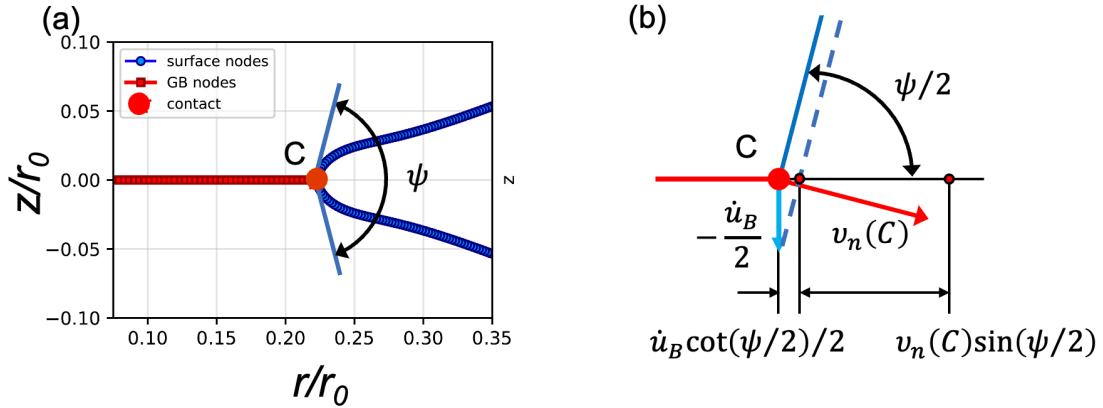


Fig. 2 Motion of the contact point C . (a) neck shape ($\gamma_{gb}/\gamma_s = 0.5$), (b) contribution of the rigid body motion and the free-surface normal velocity.

Suo [42] introduced a separate kinetic law for the motion of surface triple junction,

where a grain boundary meets surface, in thermal grooving. In addition to the surface motion, Eq. (17), we assume the contact radius is further modified by a driving force to maintain the equilibrium dihedral angle

$$\dot{c} = M_{tj} \left(2\gamma_s \cos \frac{\psi}{2} - \gamma_{gb} \right) \quad (20)$$

where M_{tj} is the junction mobility. The driving force is the sum of the surface tensions and is zero at the equilibrium dihedral angle. By introducing Eq. (20), we allow non-equilibrium dihedral angle in the shape evolution during sintering. Enforcing a fixed equilibrium dihedral angle ψ_{eq} , which is often adopted in sintering simulations, implicitly assumes an infinite junction mobility. We chose $\gamma_s M_{tj} \propto v_n(C)$. The deviations from the equilibrium angle are relaxed dynamically through Eq. (20).

4. Results

4.1 Diffusion flux map

In the BEM formulation, the chemical potential at an internal point (r, z) can be evaluated from the boundary integral representation. Its gradient was then calculated, and the diffusion flux of atoms was visualized as a vector field according to Eq. (1). The resulting flux map is shown in Fig. 3. The lengths of arrows are proportional to the logarithm of the flux velocity at that point. In the early stage, the diffusion flux is confined to regions near grain boundary and the neck. The vertical arrows along the contact area indicate the rigid body motion by densifying mechanism. The arrows from the spherical surface are directed inward, inflect, and point outward toward the neck. Fluxes from both grain boundary and spherical surface turn to the neck surface. The contact radius, then, increases by these outward fluxes (Fig. 3 (a) and (b)). The center-to-center approach of the upper and the lower particles is illustrated in Fig. 3 (b). This rigid body motion gives the shrinkage u_B . The figure also shows the neck shape is different from that expected from the sphere tangency approximations. The pair length shrinks due to the rigid body motion in the initial stage. It decreases further by the non-densifying diffusional flux in the final stage (Fig. 3 (d)).

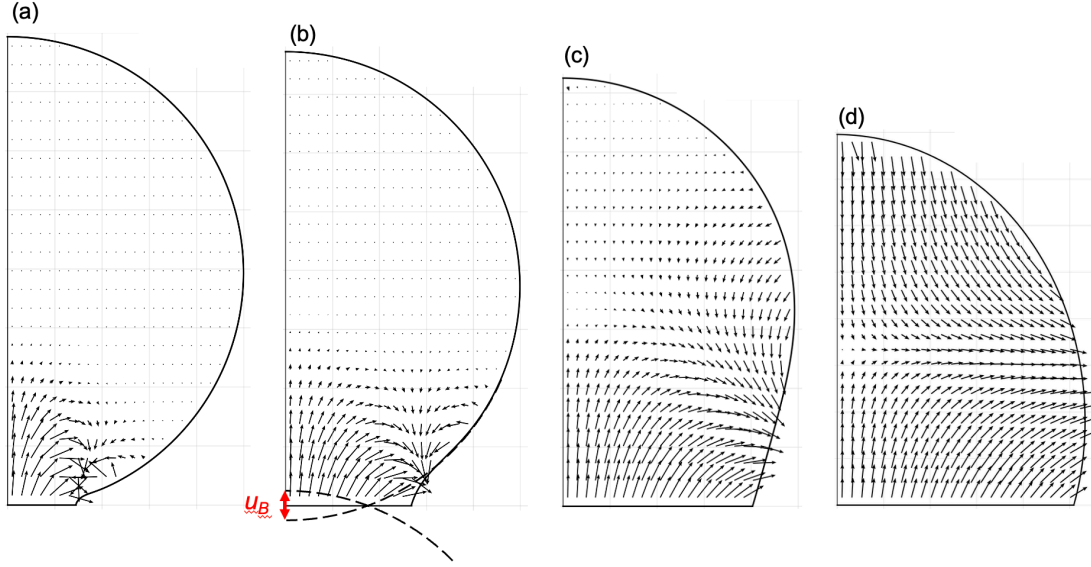


Fig. 3 Diffusion flux map in sintering of spherical particles at $\gamma_{gb}/\gamma_s = 0.5$. (a) $c/r_0 = 0.29$, $t^* = 5.5 \times 10^{-5}$, $L/2r_0 = 0.99$, $\dot{u}_B/2r_0 = 137$, (b) $c/r_0 = 0.53$, $t^* = 1.4 \times 10^{-3}$, $L/2r_0 = 0.97$, $\dot{u}_B/2r_0 = 19.5$ (c) $c/r_0 = 0.81$, $t^* = 0.018$, $L/2r_0 = 0.91$, $\dot{u}_B/2r_0 = 3.48$, (d) $c/r_0 = 1.02$, $t^* = 0.15$, $L/2r_0 = 0.80$, $\dot{u}_B/2r_0 = 0.52$.

4.2 Contact radius as a geometrical state parameter

The contact radius, evolved from the initial value of $c_0/r_0 = 0.1$, is plotted as a function of the dimensionless time in Fig. 4.

$$t^* = \frac{\gamma_s D_B \Omega}{k T r_0^3} t \quad (21)$$

The physical time t necessary to reach the particle shape at a dimensionless time t^* in Fig. 4 can be calculated by substituting parameter values, γ_s , D_B , and r_0 , into Eq. (21). It increases with r_0^3 consistent with Herring's scaling law for bulk diffusion [41]. The growth of the contact radius, or the neck growth, is often approximated in the form

$$(c/r_0)^m = \beta t^* \quad (22)$$

The slope of curves in Fig. 4 indicates the exponent m . In the initial stage, it varies from 4 to 5 in accordance with the classical theory for bulk diffusion [1, 28]. The

exponent increases further in the later stage, toward infinity at the equilibrium. We use c/r_0 as a geometrical state parameter of sintering hereafter. We provide effective curvature, sintering force, dimensionless geometric factor, and relative velocity as functions of c/r_0 , thereby, the dynamics of sintering can be predicted from the knowledge of particles geometry. This relation can be the basis for incorporating the sintering mechanics into simulations such as discrete element method, Monte Carlo method, and phase field method.

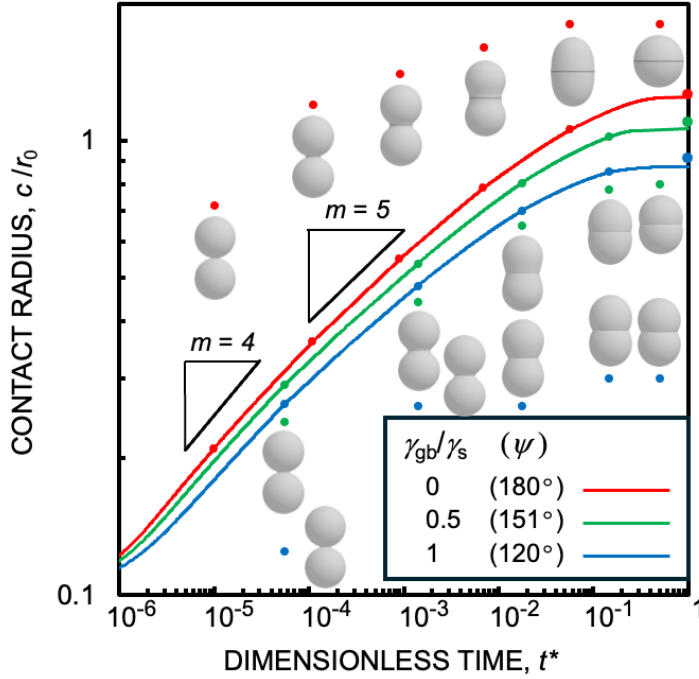


Fig.4 Contact radius as a function of dimensionless time.

4.3 Sintering force

The effective curvature κ^* , Eq. (15), is plotted as a function of c/r_0 in Fig. 5. It decreases with the neck growth analogously with the neck curvature. Since the effective curvature depends on the boundary condition on free surface, it is lower than the neck curvature. Two touching particles reach the final equilibrium state, where the particle with the initial radius r_0 becomes a truncated sphere of radius r' with the contact radius c' . The effective curvature becomes $\kappa^* = 2/r'$ at the equilibrium. r'/r_0 and c'/r' are given as functions of dihedral angle [44]. Filled circles in Fig. 5 indicate the equilibrium states. The effective curvature is used to calculate the sintering force.

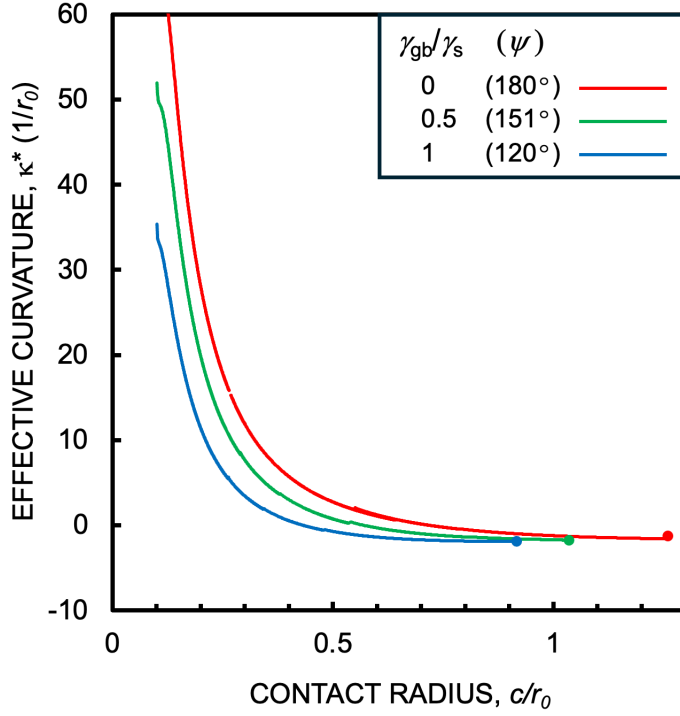


Fig. 5 Effective curvature as a function of contact radius.

The chemical potential and the corresponding normal traction σ_n on the contact depends on the boundary conditions on the free surface and the contact plane. The stress distribution on the circular contact area in Fig. 6 (a) exhibits a relatively flat shape near the center, $r/c \ll 1$, and increases steeply at $r/c \rightarrow 1$. This stress distribution is an intrinsic characteristic of the sintering by bulk diffusion [36-38] and approximated by

$$\sigma_n \approx -\frac{3}{2} \left(\gamma_s \kappa_{neck} - \frac{F_c}{A_c} \right) \sqrt{1 - \left(\frac{r}{c} \right)^2} + \gamma_s \kappa_{neck}$$

The integral of stress is equal to the force F_c acting on the contact, Eq. (5). In contrast, the stress distribution is parabolic in the sintering by grain boundary diffusion [1, 3] (Fig. 6 (b)). It is given as

$$\sigma_n = -2 \left(\gamma_s \kappa_{neck} - \frac{F_c}{A_c} \right) \left(1 - \left(\frac{r}{c} \right)^2 \right) + \gamma_s \kappa_{neck}$$

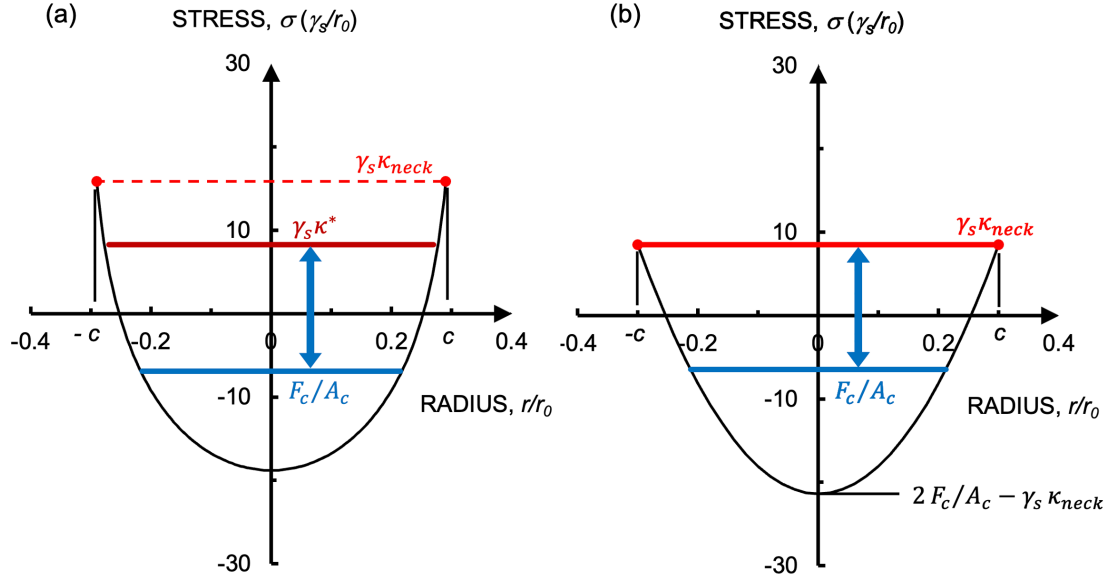


Fig. 6 Stress/chemical potential distribution on the contact area. (a) sintering by bulk diffusion ($c/r_0 = 0.3$, $\gamma_{gb}/\gamma_s = 0.5$), (b) sintering by grain boundary diffusion ($c/r_0 = 0.3$, $\gamma_{gb}/\gamma_s = 0.5$, $\delta D_{gb}/\delta D_s = 1$).

The sintering force, Eq. (14), is defined as the difference in chemical potentials between the effective curvature $\gamma_s \kappa^*$ and the average compressive stress F_c/A_c on the contact area as illustrated in Fig. 6 (a). The sintering stress is plotted as a function of the contact radius in Fig. 7. It exhibits a broad peak around $c/r_0 \approx 0.3$. The sintering force decreases toward zero at the equilibrium state. The peak height decreased with increasing γ_{gb}/γ_s .

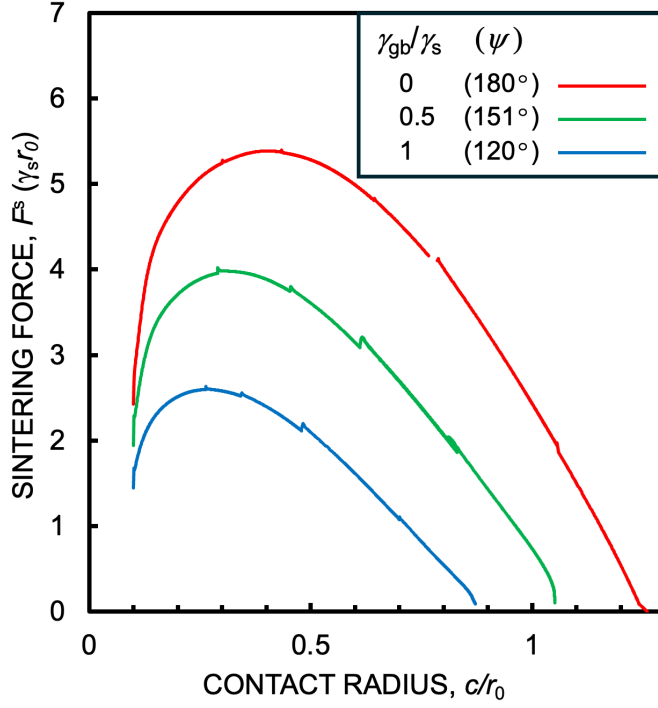


Fig. 7 Sintering force as a function of contact radius.

4.4 Relative velocity of particles

The dimensionless geometric factor g^* is plotted as a function of the contact radius in Fig. 8. The geometric factor is around 1.2 at $c_0/r_0 = 0.1$ and decreases slightly with increasing the contact radius. At the equilibrium, a particle becomes a truncated sphere of radius r' with the contact radius c' . For the dihedral angle of 180° , the particle will be a hemisphere, $c' = r' = 2^{1/3}r_0$. The dimensionless geometric factor is $g^* = 2\pi - 3/16 \approx 0.950$.

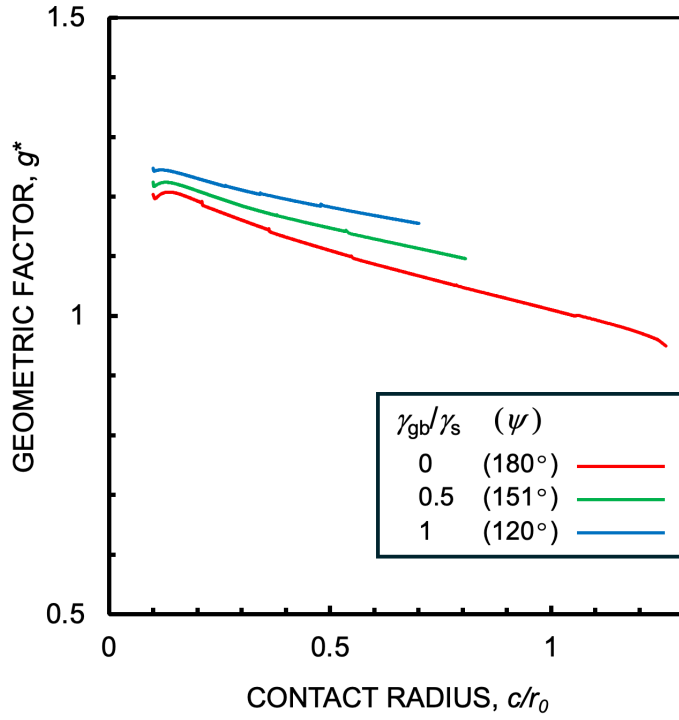


Fig.8 Relationship between the dimensionless geometric factor and contact radius.

The relative velocity, Eq. (13), is driven by the sintering force and inversely proportional to c^3 . The relation between relative velocity and the contact radius is shown in Fig. 9. As the sintering force is approximately constant near the broad peak ($0.25 < c/r_0 < 0.5$), the relative velocity decreases with $-(c/r_0)^3$ in this region. The relative velocity decreases steeply in the later stage, and the shrinkage stops when the sintering force becomes zero at the equilibrium.

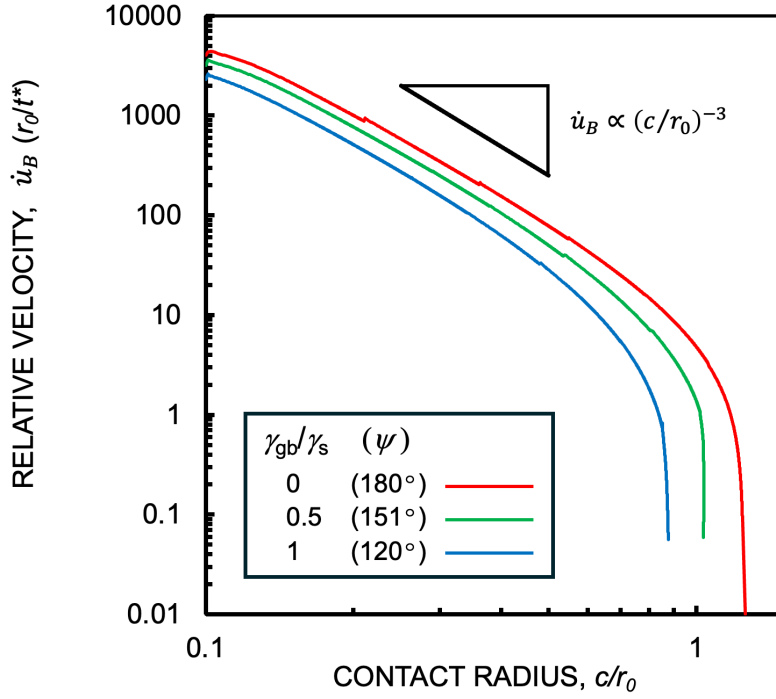


Fig. 9 Relation between relative velocity and contact radius.

Figure 10 illustrates the shrinkage as a function of contact radius. The solid line represents the distance between mass centers ΔR in Fig. 1. The broken line represents the rigid body motion u_B . The chain line corresponds to the pair length ΔL . In the sintering only by bulk diffusion, the shrinkage is caused by the rigid body motion in the early stage $c/r_0 < 0.5$. The difference between ΔR and u_B indicates the contribution of the non-densifying diffusion flux to the shift of mass centers. It is very small and can be seen only in the later stage. The non-densifying diffusion flux plays an important role in the shape evolution of particles in the final stage near the equilibrium as illustrated in Fig. 3 (d). The shrinkage ΔL defined by the pair length becomes much larger than u_B in the final stage.

If the source of matter filling in the neck is the grain boundary, the center-to-center approach is related to the contact area. Assuming a sphere tangency relation and conservation of volume gives [2, 45]

$$\frac{u_B}{r_0} \approx \frac{1}{2} \left(\frac{c}{r_0} \right)^2$$

The dotted line in Fig. 10 shows this relationship. Starting from the initial contact radius

$c_0/r_0 = 0.1$, the shrinkage curve approaches to this sphere tangency model asymptotically. However, the slope based on the simplified assumption agrees only at $c/r_0 \sim 0.3$, where the sintering force is regarded as a constant due to the broad peak.

The amount of the final shrinkage decreases with increasing γ_{gb}/γ_s as shown in Fig. 11.

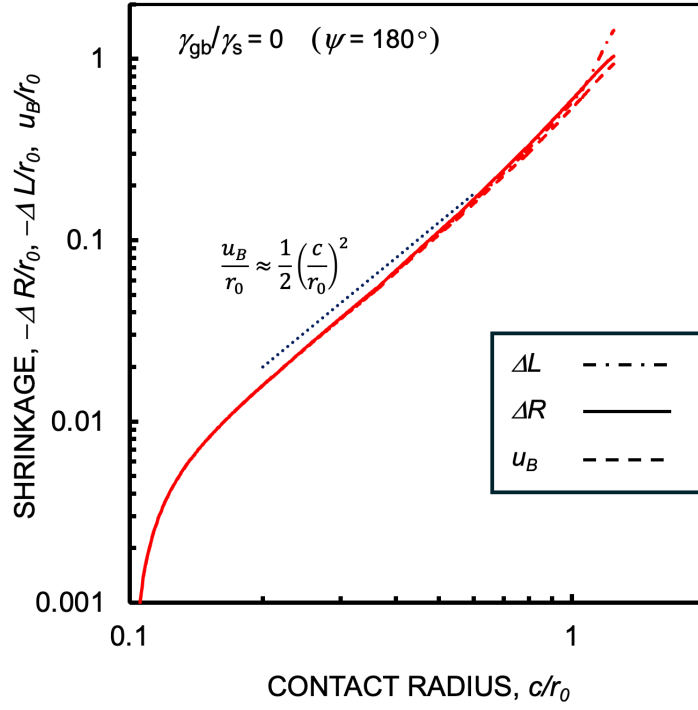


Fig. 10 Shrinkages (ΔL , ΔR , and u_B) as functions of the contact radius.

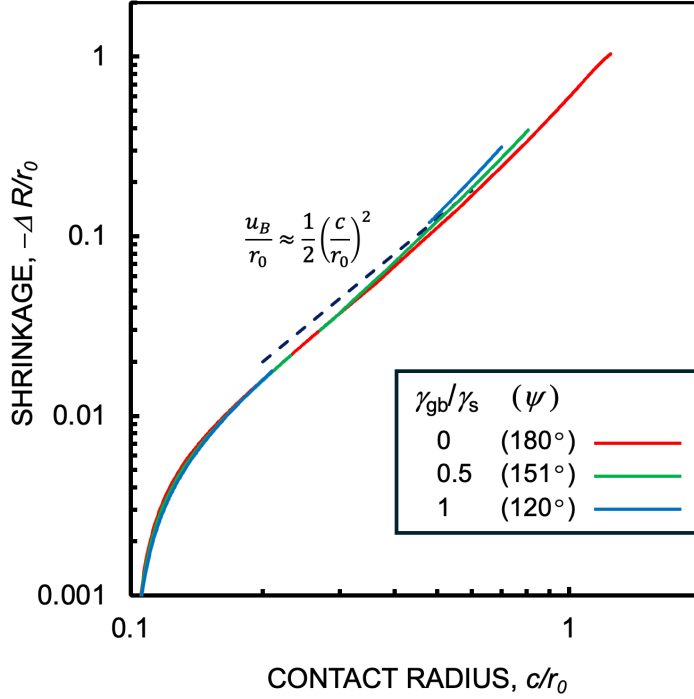


Fig. 11 Shrinkage ΔR as a function of the contact radius.

5. Discussion

When the grain boundary acts as the perfect sink of vacancy, the densification mechanisms by bulk diffusion and grain boundary diffusion take place simultaneously. In Ashby's attempt to construct the sintering mechanism diagrams [26, 27], the densifying mechanisms by bulk diffusion and grain boundary diffusion were regarded as independent. This is an approximation suitable for understanding each fundamental mechanism, thereby, we adopted it as the first step in this paper. The relative velocity between two particles in the sintering by grain boundary diffusion is described as [3-6]

$$\dot{u}_{gb} = -\frac{8\Omega\delta D_{gb}}{kT\pi c^4} F_{gb}^s \quad (23)$$

$$F_{gb}^s = \gamma_s \kappa_{neck} A_c + \gamma_s L_c \sin(\psi/2) \quad (24)$$

The sintering force for bulk diffusion, Eq. (14), is defined analogously to that for grain boundary diffusion. It is simply obtained by replacing the neck curvature κ_{neck} by the effective curvature κ^* . Both F_B^s and F_{gb}^s are illustrated as functions of c/r_0 in Fig. 7 and Fig. 11 in [9], respectively. The peak height of F_B^s is lower than F_{gb}^s ,

because the effective curvature κ^* is lower than the local curvature at the neck κ_{neck} . The peak width of F_B^s is wider than that of F_{gb}^s . The peak position of F_{gb}^s locates at $c/r_0 \approx 0.2$, while that of F_B^s locates around $c/r_0 \approx 0.3$.

If $F_B^s \approx F_{gb}^s$, the comparison of Eq. (13) with Eq. (23) leads to

$$\frac{\dot{u}_B}{\dot{u}_{gb}} \propto \frac{cD_B}{\delta D_{gb}} \quad (25)$$

The contribution of bulk diffusion flux was assumed to be proportional to the bulk diffusion coefficient multiplied by an appropriate geometric scaling factor l . It is equivalent to assuming an effective diffusion width l for bulk diffusion. Equation (25) indicates $l \sim c$ in agreement with the prediction by Wilson and Shewmon [30] and Maximenko and Olevisky [38]. The contribution of bulk diffusion to the shrinkage is small at the initial stage and increases with the contact radius in the later stage.

The equation of motion by grain boundary diffusion, Eq. (23), can be converted into a non-dimensional form by introducing a dimensionless time t^*

$$t^* = \frac{\gamma_s \delta D_{gb} \Omega}{kT r_0^4} t \quad (26)$$

The physical time t necessary to reach a particular state increases with r_0^4 consistent with Herring's scaling law for grain boundary diffusion [43]. The relative velocity is, then, proportional to r_0^{-4} and r_0^{-3} for grain boundary diffusion and bulk diffusion, respectively. For a given c/r_0 , the contribution of bulk diffusion to the relative velocity increases with increasing the particle size,

$$\frac{\dot{u}_B}{\dot{u}_{gb}} \propto \frac{r_0 D_B}{\delta D_{gb}} \quad (27)$$

Here, we must emphasize that the sintering mechanisms by bulk diffusion and grain boundary diffusion are not independent. Eadie, Wilkinson, Weatherley [36] and Ross, Miller, Weatherly [37] demonstrated an approach for the coupled bulk and grain boundary diffusions, although they have not analyzed the micromechanical aspect of the sintering, i.e., the sintering force. As the next step, it is necessary to extend our micromechanical analysis to the sintering coupled with surface diffusion, grain boundary diffusion, and bulk diffusion.

6. Conclusion

The objective of this paper was to identify the origin of the sintering force in sintering by bulk diffusion. The Laplace equation for diffusion potential was solved by decomposing the solution into two subproblems, one for non-densifying solution and the other for densifying solution. The integral of the non-densifying solution at the contact provides an effective curvature. As the grain boundary is assumed the perfect source/sink of vacancies, the stress distribution on the contact between two particles is obtained from the chemical potential of densifying problem. The integral of stress on the contact is given by the force balance and is simply calculated from the surface tension. The sintering force arises from the difference between the chemical potential related to the effective curvature and that related to the average compressive stress on the contact. The sintering force for bulk diffusion was obtained analogously to that of grain boundary diffusion. It is given by replacing the neck curvature by the effective curvature.

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Declaration of generative AI and AI-assisted technologies in the manuscript preparation process

During the preparation of this work, the authors used ChatGPT (OpenAI) and Claude (Anthropic) to assist with drafting selected Python code segments, identifying possible programming errors, improving code structure, and refining the language of the manuscript. After using these tools, the authors critically reviewed, revised, and edited all generated output as needed and take full responsibility for the content of the published article.

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Figure captions

Fig. 1 Sintering of two spherical particles. The black dot inside a particle indicates the mass center. The distance of mass centers, R , and the pair length, L , are defined in the figure.

Fig. 2 Motion of the contact point C . (a) neck shape ($\gamma_{gb}/\gamma_s = 0.5$), (b) contribution of the rigid body motion and the free-surface normal velocity.

Fig. 3 Diffusion flux map in sintering of spherical particles at $\gamma_{gb}/\gamma_s = 0.5$. (a) $c/r_0 = 0.29$, $t^* = 5.5 \times 10^{-5}$, $L/2r_0 = 0.99$, $\dot{u}_B/2r_0 = 137$, (b) $c/r_0 = 0.53$, $t^* = 1.4 \times 10^{-3}$, $L/2r_0 = 0.97$, $\dot{u}_B/2r_0 = 19.5$ (c) $c/r_0 = 0.81$, $t^* = 0.018$, $L/2r_0 = 0.91$, $\dot{u}_B/2r_0 = 3.48$, (d) $c/r_0 = 1.02$, $t^* = 0.15$, $L/2r_0 = 0.80$, $\dot{u}_B/2r_0 = 0.52$.

Fig.4 Contact radius as a function of dimensionless time.

Fig. 5 Effective curvature as a function of contact radius.

Fig. 6 Stress/chemical potential distribution on the contact area. (a) sintering by bulk diffusion ($c/r_0 = 0.3$, $\gamma_{gb}/\gamma_s = 0.5$), (b) sintering by grain boundary diffusion ($c/r_0 = 0.3$, $\gamma_{gb}/\gamma_s = 0.5$, $\delta D_{gb}/\delta D_s = 1$).

Fig. 7 Sintering force as a function of contact radius.

Fig.8 Relationship between the dimensionless geometric factor and contact radius.

Fig. 9 Relation between relative velocity and contact radius.

Fig. 10 Shrinkages (ΔL , ΔR , and u_B) as functions of the contact radius.

Fig. 11 Shrinkage ΔR as a function of the contact radius.