Modeling dislocation glide and lattice friction in Mg_2SiO_4 wadsleyite in conditions of the Earth's transition zone

Supplementary section: Thermal activation of glide of collinear dissociated dislocations

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Introduction

Within the thermally activated regime, the glide velocity of dislocations is governed by the nucleation and propagation of unstable kink-pairs on the dislocation lines under the action of resolved shear stress. This atomic-scale process can be captured by the critical nucleation enthalpy associated with it. These calculations are parametrized by the dislocation core structures and their lattice friction given by the Peierls potentials. The latter is calculated by making use of a generalized Peierls-Nabarro model (Peierls 1940; Nabarro 1947) which itself relies on the γ-surfaces of the potential slip planes in wadsleyite at 15 GPa (Metsue et al. 2010).

Kink-pair nucleation on collinear dissociated screw dislocations

Kink-pair modeling based on the elastic interaction model of Koizumi et al. (1993) and adapted to collinear dissociated dislocations (Ritterbex et al. 2015)

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as they exist in wadsleyite allows to calulate the critical nucleation enthalpies related to glide. However, kink-pair nucleation processes must occur on both partials for the complete dislocation to move. This can happen in several different ways as illustrated in Fig. 1 of the main article. A kink-pair on each partial may simultaneously nucleate so that they coincide along the partials: "correlated" nucleation (Fig. 1a). The nucleation process may also occur independently on both partials to which we will refer to as "uncorrelated" nucleation. Two end-member types of uncorrelated nucleation processes are possible: the outward motion of the leading partial as a first unit step, followed by the inward motion of the trailing partial (Fig 1b) or the inward motion of the trailing partial as a first unitstep followed by the outward motion of the leading partial (Fig. 1c).

Correlated nucleation can occur at $0 < \tau \leq \tau_p$, whereas uncorrelated nucleation of kink-pairs exhibit lower nucleation enthalpies but is only possible at $\tau \geq \tau_c$, since the absolute energy level of the next Peierls valley associated with the inward or outward motion of one partial, is higher than the orginal valley as a consequence of a significant change in equilibrium stacking fault width d and the subsequent change in stacking fault energy and elastic interaction energy between both partials (Möller 1978; Takeuchi 1995). The critical stress τ_c therefore is fully determined by the properties of the dissociated dislocation core structure.

The enthalpy variation associated with the mechanism for those kink-pair nucleation processes can generally be described by:

$$\Delta H = \Delta E_{elastic} + c_i \Delta P_p + \Delta W_{sf} + c_i W_p \tag{1}$$
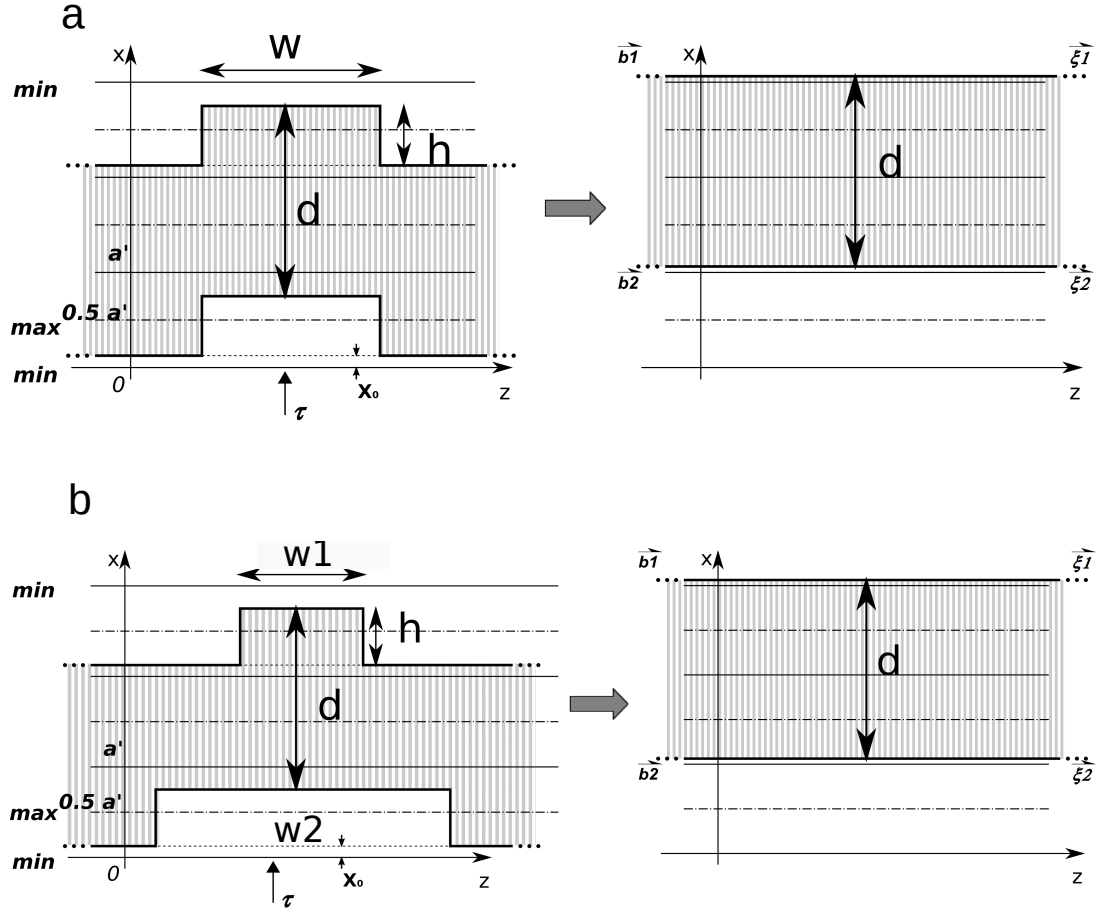
where

Figure S1: Correlated kink-pair nucleation on collinear dissociated dislocations with equilibrium stacking fault width d. a) Correlated kink-pair nucleation on both partials along the dislocation lines in the low stress end member case. b) Correlated kink-pair nucleation along both partial lines where small changes in both stacking fault and elastic interaction energy between the partials are allowed to occur

$$\Delta E_{elastic} = \Delta E_{\xi_1} + \Delta E_{\xi_2} + \Delta E_{\xi_1,\xi_2} \qquad (2)$$

The enthalpy variation ΔH is due to the change in elastic energy $\Delta E_{elastic}$, the change in stacking fault energy $\Delta W_{sf} = \pm\gamma hw$, where γ is equal to the equilibrium stacking fault energy, the variation in Peierls energy ΔP_p and the

plastic work ΔW_p under the action of the resolved shear stress τ. In Eq. 1, $c_i = c_u = 1$ for uncorrelated and $c_i = c_c = 2$ for correlated kink-pair nucleation. We want to note that Eq. (1) is equal to Eq. (2) of the main article.

All variations in the elastic energy $\Delta E_{elastic}$ (Eq. 2), between two consecutive dislocation configurations divided into segments, are calculated considering piecewise straight line segments within an isotropic elastic continuum by using the coplanar elastic interaction formalism formulated by Hirth and Lothe (1982). In here, the change in elastic interaction energy between the two partial dislocation lines is given by $\Delta E_{\xi_1, \xi_2}$. The overall variation in elastic energy ΔE_{ξ_n} (Eq. 2), is given by the total change in elastic interaction energy and the change in self-energy of the line(s). These functions depend on the heights of and the widths between kink-pairs, but also on the change in absolute self energy of the partial dislocations due to the creation of new line segments (see Fig. S1). The latter is expressed in a fixed cut-off radius ρ (Hirth and Lothe 1982; Koizumi et al. 1993). Following previous work (Koizumi et al. 1993; Carrez et al. 2009; Ritterbex et al. 2015), we consider a cut-off radius of 10% of the width of a partial dislocation ($\rho = 0.1\xi_n$) in order to introduce the dependency of the change in self energy of the partials on the choice of slip system. The choice of ρ may therefore affect the absolute value of the critical nucleation enthalpy but will not influence the relative difference with respect to different slip systems.

The formation of a kink-pair on one partial leads as well to a variation in the Peierls energy dependent on the Peierls potential V_p (Eq. 1). The applied resolved shear stress τ will rigidly force the dislocation into a new quasi-equilibrium position x_0 within the crystal lattice :

$$\Delta P_p = \int_{x_0}^{x_0+h} V_p dx + \frac{w}{2} \left[V_p \left(x_0 + h \right) - V_p \left(x_0 \right) \right] \tag{3}$$

The underlying assumption is that each equivalent partial dislocation has to overcome half of the complete Peierls potential V_p (Eq. 1 of the main article). The first part on the right hand side of Eq. 3 describes the energy associated with kinks crossing the potential whereas the second term accounts for the energy related to the position of the nucleated line segment w in the crystal.

Correlated kink-pair nucleation: low stress regime

End-member case in the low stress regime: $\tau \to 0$

Kink-pair nucleation in the end-member case $\tau \to 0$, relies on the nucleation of two strictly identical rectangular kink-pairs on both partial dislocations. The reason is that the work performed by the resolved shear stress is insufficient to allow for the energy cost related to a change in the stacking fault. This means that all kinks exhibit an equivalent height h and that both kink-pairs consist of two kinks separated by an equivalent width w (Fig. S1a). The change in (equilibrium) stacking fault width d associated with this type of kink-pair nucleation is negligable as can be seen in Fig. S1a. The variation in enthalpy ΔH_c associated with correlated nucleation of two identical kink-pairs on both partials has been derived analytically and is equal to:

$$\Delta H_c = \Delta E_{\xi_1} + \Delta E_{\xi_2} + \Delta E_{\xi_1,\xi_2} + 2\Delta P_p + 2\Delta W_p \tag{4}$$

where the change in elastic energy ΔE_{ξ_n} of a screw partial ξ_n is given by:

$$\begin{aligned}
\Delta E_{\xi_n}(h,w) = \frac{\mu b_p^2}{2\pi} \Bigg(& \sqrt{w^2 + h^2} - w - h + w \log \frac{2w}{w + \sqrt{w^2 + h^2}} \\
& -\frac{1}{1-\nu}\left(w - \sqrt{w^2+h^2} + h\log\frac{h+\sqrt{w^2+h^2}}{w} - h\log\frac{h}{e\rho}\right)\Bigg)
\end{aligned} \tag{5}$$

where μ is the shear modulus, ν is the Poisson ratio, b_p is the modulus of the partial Burgers vector and ρ is equal to a fixed cut-off radius reflecting a change in absolute self energy of the partials as a consequence of the creation of the edge kink segments. The height h of the kinks and the width w between a pair of kinks describe the geometry of the kink-pair(s). The change in elastic interaction $\Delta E_{\xi_1,\xi_2}$ between the partial dislocations is mainly due to the elastic interaction between the kinks of both lines and has been derived as :

$$\Delta E_{\xi_1,\xi_2} = \Delta E_k = \frac{\mu b_p^2}{2\pi\,(1-\nu)} h \log \frac{d}{d-h} \tag{6}$$

where d is equal to the equilibrium stacking fault width. The plastic work ΔW_p performed by the resolved shear stress τ on one partial and the change in Peierls energy ΔP_p due to kink-pair formation on a partial are given in the main article. By solving $\partial H/\partial h = \partial H/\partial w = 0$, for a given stress τ, the critical nucleation enthalphy ΔH_c^{crit} as a function of the critical kink-pair geometry, h^{crit} and w^{crit}, can be found as the saddle point configuration of the respective total enthalpy variation ΔH_c. Generally, the height h of all kinks, in the end-member case where $\tau \to 0$, is equal to the full period a' of the Peierls potential.

Low stress regime: $\tau > 0$

Kink-pair nucleation in the end-member case at low stress conditions is based on the nucleation of two strictly identical kink-pairs on both partials. However, the work done by the applied resolved shear stress in the low stress regime can be sufficient to account for the energy variation related to small changes in the stacking fault as in illustrated in Fig. 1b by correlated formation of two geometrically different kink-pairs on both partials. Since we are still in the low stress regime, the critical height is taken to be fixed as $h^{crit} = a'$ for $\tau \to 0$

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and the widths w_1 and w_2 between the kink-pairs on both partials 1 and 2 respectively are now taken to be the free geometrical variables (Fig. 1b). The critical nucleation enthalpy ΔH_{cc} associated with this nucleation processes is equal to:

$$\Delta H_{cc} = \Delta E_{\xi_1} + \Delta E_{\xi_2} + \Delta E_{\xi_1,\xi_2}^s + 2\Delta P_p + 2\Delta W_p \tag{7}$$

where $\Delta E_{\xi_1,\xi_2}^s = \Delta E_{\xi_1,\xi_2} + \Delta W_s$. Here, ΔW_s is equal to two opposite contributions: the change in stacking fault energy and the along going variation in interaction energy between the partial line segments:

$$\Delta W_s = \frac{\mu b_p^2}{2\pi} \left(-2a' - 2\sqrt{w^2 + (d-a')^2} - w \log \frac{\sqrt{w^2 + (d-a')^2} - w}{\sqrt{w^2 + (d-a')^2} + w} \right.$$
$$\left. +2\sqrt{w^2 + d^2} + w \log \frac{\sqrt{w^2 + d^2} - w}{\sqrt{w^2 + d^2} + w} \right) - 2\gamma a' w \tag{8}$$

where d is the equilibrium stacking fault width and $w=1/2(w_2 - w_1) > 0$. The change in elastic interaction $\Delta E_{\xi_1,\xi_2}$ between the partial dislocations is mainly due to the elastic interaction between the kinks of both lines and has been derived as:

$$\Delta E_{\xi_1,\xi_2} = \frac{\mu b_p^2}{2\pi(1-\nu)} \left(2\sqrt{w^2 + d^2} - d \log \frac{\sqrt{w^2 + d^2} + d}{\sqrt{w^2 + d^2} - d} \right.$$
$$-\sqrt{w^2 + (d+a')^2} + 1/2(d+a') \log \frac{\sqrt{w^2 + (d+a')^2} + (d+a')}{\sqrt{w^2 + (d+a')^2} - (d+a')}$$
$$\left. -\sqrt{w^2 + (d-a')^2} + 1/2(d-a') \log \frac{\sqrt{w^2 + (d-a')^2} + (d-a')}{\sqrt{w^2 + (d-a')^2} - (d-a')} \right) \tag{9}$$

In Eq.(7), ΔE_{ξ_n} is defined as in Eq. (5).

[100](010) *screw dislocation*

In case of the [100](010) screw dislocation, the critical nucleation enthalpies calculated at low stress conditions using Eq. (7) are equal to the critical nucleation enthalpies in the end member case at low stress using Eq. (4), on the condition that $\Delta E_k{=}0$ (Eq. 6). This implies that the use of linear elasticity overestimates the kink-kink interaction between the rectangular kink-pairs on both partials in the end member case of the low stress regime, since small changes in the stacking fault are able to reduce the kink-kink interactions. As a consequence, the enthalpy variation associated with correlated kink-pair nucleation on the [100](010) screw dislocations are finally taken to be equal to Eq. (4) with $\Delta E_{\xi_1,\xi_2}{=}E_k{=}0$. This is generally the case for dissociated dislocations that exhibit low to intermediate stacking fault widths (or high and intermediate stacking fault energies) of approximately $a' \leq d \leq\ 3a'$.

$\frac{1}{2}\langle 111 \rangle\{101\}$ *screw dislocation*

The situation is different in the case of the $\frac{1}{2}\langle 111 \rangle\{101\}$ screw dislocation. This is mainly due to the difference in ΔW_s (Eq. 7 and 8) between the [100](010) and $\frac{1}{2}\langle 111 \rangle\{101\}$ screws in case of small changes in the stacking fault at low stress. For the [100](010) screw dislocation, the change in stacking fault energy more or less compensates the along going variation in interaction energy between the partial lines. For widely dissociated dislocations, where approximately $d \geq 3a'$, both terms have significant different weights: the change in stacking fault energy becomes more important than the variation in elastic interaction energy between the partials, despite the low stacking fault energies. This is due to the fact that the variation in interaction energy between widely separated partial lines is unsignificantly small. It means that stacking fault changes for widely dissociated dislocations helps the nucleation process to occur by a decrease in the critical activation enthalpy at low stress. Therefore, the enthalpy variation

associated with correlated kink-pair nucleation on the $1/2\langle111\rangle\{101\}$ screws are finally taken to be equal to Eq. 7 in order to caption the aforementioned role of the stacking fault.

Uncorrelated kink-pair nucleation: high stress regime

The alternative to glide of dissociated dislocations is the motion of the partials as a result of uncorrelated kink-pair nucleation. These processes typically govern kink-pair nucleation on dissociated dislocatons in the high stress regime since this type of mechanism is characterized by an explicit change in the equilibrium stacking fault width. The kink-pair model in this case relies on the nucleation of a rectangular kink-pair of height h and width w on one partial dislocation at the time. The variation in enthalpy ΔH_{u_n} associated with one unit step of uncorrelated kink-pair nucleation can be described as follows:

$$\Delta H_{u_n} = \Delta E_{\xi_n} + \Delta E_{\xi_1,\xi_2} + \Delta W_{sf} + \Delta P_p + \Delta W_p \tag{10}$$

where the variation in interaction energy $\Delta E_{\xi_1,\xi_2}$ between the partials is described as the change in elastic interaction energy between both dislocation lines as a consequence of the kink-pair formation on either the leading or the trailing partial:

$$\Delta E_{\xi_1,\xi_2} = \frac{\mu b_p^2}{4\pi}\left(\pm 2h - 2\sqrt{w^2 + d_f^2} - w\log\frac{\sqrt{w^2 + d_f^2} - w}{\sqrt{w^2 + d_f^2} + w}\right.$$
$$\left. + \ +2\sqrt{w^2 + d_i^2} + w\log\frac{\sqrt{w^2 + d_i^2} - w}{\sqrt{w^2 + d_i^2} + w}\right) \tag{11}$$

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This expression is dependent on the precise mechanism of a unit step such that d_i and d_f correspond to the initial and final stacking fault width between both partial dislocations respectively during nucleation as shown in Fig. 1b and c of the main article. ΔW_{sf} is equal to the change in stacking fault energy $\pm \gamma h w$ and balances as such the variation in elastic interaction energy $\Delta E_{\xi_1, \xi_2}$.

Parametrization of the dislocation mobility

Dislocation mobilities can be described by the dislocation glide velocities with respect to the different slip systems (Dorn and Rajnak 1964; Guyot and Dorn 1967; Möller 1978). The velocity is a function of the stress dependent critical nucleation rate of kink-pairs. The latter depends on the critical nucleation enthalphy ΔH^{crit} and critical kink-pair geometry on the dislocation lines. The dislocation velocity for $\tau \leq \tau_c$ is equal to

$$v_c \left(\tau, T \right) = a' J_c \left(\Delta H_c^{crit} \right) \tag{12}$$

where the nucleation rate for correlated kink-pair formation J_c is given by

$$J_c = \nu_0 \frac{b_p}{w^{crit} \left(\tau \right)} \frac{L}{2 b_p} \exp \left(-\frac{\Delta H_c^{crit} \left(\tau \right)}{k_b T} \right) \tag{13}$$

The dislocation velocity for $\tau \geq \tau_c$ is due to both correlated and uncorrelated kink-pair nuleation and given by [Möller, 1978]:

$$v_{c+u} \left(\tau, T \right) = \frac{1}{2} a' \left[J_c \left(\Delta H_c^{crit} \right) + J_u \left(\Delta H_u^{crit} \right) \right] \tag{14}$$

where the nucleation rate for uncorrelated kink-pair formation J_u is given by

$$J_u = \nu_0 \frac{b_p}{w^{crit}(\tau)} \frac{L}{b_p} \left(\frac{\tau - \tau_c}{\tau} \right) \exp \left(-\frac{\Delta H_u^{crit}(\tau)}{k_b T} \right) \tag{15}$$

where the pre-exponential factor $(\tau - \tau_c)/\tau$ has been introduced to guarantee the continuity between both velocity solutions v_c and v_{c+u}. It relies on the assumption that the dislocation velocity v_{c+u} at $\tau = \tau_c$ has to be strictly equal to that of v_c.

The dislocation mobility depends as well on the evolution of the critical kink-pair geometry (Eq. 12, 13, 14 and 15). Under low stress conditions, the critical height h^{crit} of a kink is about equal to the Peierls periodicity a' and decreases with increasing stress. The critical width rapidly converges to finite values with increasing stress but diverges when the resolved shear stress goes to zero. Therefore, the critical kink-pair width needs to be truncated at low stresses with respect to the typical average length $L = 1/\sqrt{\rho_m}$ (where ρ_m is equal to the dislocation density) of the partial dislocation lines. The value w^{crit} for the $[100](010)$ screw dislocations converges rapidly within $0.1\tau_p$ to a value of $\sim 8b_p$. The width w^{crit} for the $1/2\langle 111\rangle\{101\}$ screw dislocations regarding uncorrelated nucleation converges within $0.2\tau_p$ to a value of $\sim 10b_p$. For correlated nucleation regarding kink-pairs exhibiting different widths, w_1^{crit} and w_2^{crit} converges within $0.02\tau_p$ to $\sim 15b_p$ and $\sim 5b_p$, respectively. Therefore, independent of slip system and kink-pair nucleation mechanisms, small values of w^{crit} are found to be converged at relatively low stresses. These small values for $w^{crit}(\tau)$ are expected for slip systems with large Peierls stresses as discussed by Philibert (1979).

References

Carrez, Ph., Ferré, D., and Cordier, P. (2009) Thermal activation of dislocation glide in MgO based on an Elastic-Interaction model of kink-pair nucleation. In IOP Conference Series: Materials Science and Engineering 3, 1-9.

Dorn, J.E., and Rajnak, S. (1964) Nucleation of kink pairs and the Peierls' mechanism of plastic deformation. Transactions of the Metallurgical Society of AIME, 230, 1052-1064.

Guyot, P., and Dorn, J.E. (1967) A critical review of the Peierls mechanism. Canadian Journal of Physics, 45, 983-1016.

Hirth, J.P., and Lothe, J. (1982) Theory of dislocations. John Wiley & Sons, New York.

Koizumi, H., Kirchner, H.O.K., and Suzuki, T. (1993) Kink pair nucleation and critical shear stress. Acta Metallurgica et Materialia, 41, 3483-3493.

Metsue, A., Carrez, Ph., Denoual, C., Mainprice, D., and Cordier, P. (2010) Plastic deformation of wadsleyite: IV Dislocation core modelling based on the Peierls-Nabarro-Galerkin model. Acta Materialia, 58, 14671478.

Möller, H.-J. (1978) The movement of dissociated dislocations in the diamond-cubic structure. Acta Metallurgica, 26, 963-973.

Nabarro, F. R. N., (1947) Dislocations in a simple cubic lattice. Proceedings of the Physical Society, 59, 256-272.

Peierls, R.E. (1940) The size of a dislocation. Proceedings of the Physical Society, 52, 34-37.

Philibert, J. (1979) In Dislocations et Déformations Plastique, Eds., P. Groh, L.P. Kubin, and J.-L. Martin, CNRS École d'été d'Yvrals (in French).

Ritterbex, S., Carrez, Ph., Gouriet, K., and Cordier, P. (2015) Modeling dislocation glide in Mg_2SiO_4 ringwoodite: Towards rheology under transition zone conditions. Physics of the Earth and Planetary Interiors, 248, 20-29.

Takeuchi, S. (1995) Glide of interacting partial dislocations in the Peierls mechanism. Philosophical Magazine A, 71(6), 1255-1263.