Computational materials science meets geophysics: dislocations and slip planes of MgO

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Abstract

We calculate the generalised stacking fault (GSF) surface energies of MgO using an interatomic potential that mimics accurately the ab initio energies, forces and stresses. Using the GSF in the framework of Peierls-Nabarro model, the properties of dislocations in MgO have been determined for its three main slip systems: $\{110\}(1\bar{1}0)$, $\{100\}(011)$ and $\{111\}(1\bar{1}0)$. The obtained Peierls stresses are in good agreement with experimental data and yields the correct dominant slip system in MgO, namely $\{110\}(1\bar{1}0)$ at low temperature and pressure.

Key words: MgO, dislocation, deformation, Peierls-Nabarro model
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1. Introduction

Magnesium oxide (MgO) is the second most abundant mineral in the lower Earth's mantle and is considered a paradigm for ionic oxides[1]. Due to its simplicity and geophysical importance, it is crucial to understand and characterize its properties under extreme conditions of pressure. The rheological properties of minerals are essential to model and explain several geophysical phenomena including the seismic anisotropy in some regions of the Earth. However, high-pressure experiments on the deformation of MgO are extremely difficult and very little information is available on its microscopic deformation under Earth's mantle conditions [2,3].

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In the theoretical description of rheology of materials usually two approaches are followed: the atomistic approach explores the microscopic properties, while the continuum one accounts for the macroscopic phenomena. But, the bridge between the two approaches is still challenge in the modeling of materials [4–6]. One key point is the determination of the dislocation properties. This is particularly true in minerals, which deform by dislocation glide and climb [2,3]. Therefore plastic behavior and anisotropy can be understood by studying the motion of dislocations in given particular planes and directions.

The purpose of this paper is to introduce some methods of computational materials science within geophysical problems. We attempt to describe quantitatively the rheology of MgO and determine the properties of its dislocations at low temperature and low pressure conditions. Here, we will use the theo-

retical framework of generalised stacking fault (GSF) surface energies and the Peierls-Nabarro (PN) model to study the dislocation structure and mobility [4,5]. The PN model combines the atomistic description of the dislocation core, which is obtained by the accurate determination of the forces close to the core as determined by GSF calculations, with the elastic contribution in the continuum. This approach has been successfully used to describe the dislocation properties of metal, intermetallic compounds and covalent systems[6]. On the other hand, to our knowledge there have been no systematic calculations of GSF surfaces of ionic systems. The effects of finite temperature and pressure and the geophysical consequences of our findings are reported separately[7].

2. Methodology

The GSF calculations are based on the determination of the energy cost (with respect to the ideal crystal) of shearing along a given direction the two halves of a crystal cut along the glide plane. MgO has a NaCl cubic structure stable over a large range of temperature and pressure. In cubic lattices, it is expected that the main slip systems are: $\{110\}(1\overline{1}0)$, $\{100\}(011)$ and $\{111\}(1\overline{1}0)$ [2]. The GSF energies of those slip systems have been obtained by using an interatomic potential, which mimics accurately the ab initio energy surfaces, as well forces and stresses [8]. The accuracy of the interatomic potential has been checked with respect to GSF ab initio calculations [7]. During the shearing process, the relaxation plays an important role. In our calculations, the atoms are allowed to relax only in the direction perpendicular to the glide plane by using the steepest descent method. Periodic boundary conditions have been applied and the size of the computational cells has been choosen in order to minimize the effects of interactions between the images of the glide plane. To this end, 18 planes have been considered in the direction perpendicular to the glide plane. No significant size effects were observed with this choice.

3. Peierls-Nabarro model and dislocation properties

Our results for the GSF surface and the restoring forces for the main slip systems of MgO are shown in Fig.1. The restoring force ($F_b(f(x))$) is determined by the derivative of the GSF with respect to the dislocation profile ($f_b(x')$) at position x' from the dislocation line.

We first consider the results for the GSF in Fig.1a. Our calculations show that the slip system $\{110\}(1\overline{1}0)$ has the lower energy barrier and its maximum value of the GSF γ_{max} is almost half of the values found for the other slip systems (see Table 1). A similar behavior can be observed for the restoring forces (Fig.1b) and their maximum values τ_{max} as can be also seen in Table 1. It should be noticed that the forces for $\{110\}(1\overline{1}0)$ are significately different from the usual sinusoidal function proposed in the original PN model. The other two slip systems,$\{100\}(011)$ and $\{111\}(1\overline{1}0)$, have close values for both γ_{max} and τ_{max}. This result is consistent with the experimental evidence that $\{110\}(1\overline{1}0)$ is the dominant slip plane in MgO at low temperature and pressure. [2,9]

Let us now analyse the properties of dislocations by using the GSF results as an input for the PN model. The continuum solution for the dislocation profile is obtained by solving the so called Peierls-Nabarro equation, which balances the restoring forces with the elastic stress [4,5]:

$$\frac{K}{2\pi}\int [\frac{d}{dx}f_b(x')]\frac{1}{x-x'}dx' = F_b(f(x)) \qquad (1)$$

where K is related to the elastic properties of the material along a given direction and b the Burgers vector of the dislocation (see Table 1). We follow the procedure in references [4,5] to numerically solve the PN equation. The dislocation density (ρ_b) is directly related to the dislocation profile as [4,5]:

$$\rho_b = \frac{d}{dx}f_b(x) \qquad (2)$$

In Fig.2, we show the dislocation profile (a) and densities (b) for planar dislocations in the three slip systems studied. For the case of dislocations in the $\{100\}(011)$ and $\{111\}(1\overline{1}0)$, the dislocation profiles

and densities are similar. This reflects the similarity in the restoring forces obtained for those slip planes. However, for the $\{110\}(1\bar{1}0)$ a very interesting behavior has been observed and the peaks in the dislocation density suggest that the full dislocation will dissociate in two partials. The summary of the parameters related to the planar dislocations in MgO is given in Table 1.

From the solution of PN model, it is possible to obtain other useful properties of dislocations: the misfit energy and the Peierls energy and stress. The misfit energy is given as a sum of all misfit energies between pair of atomic planes [4,5]:

$$W(u) = \sum_{m=-\infty}^{+\infty} a'\gamma_{GSF}[f_b(ma' - u)] \quad (3)$$

where a' is the spacing of atomic planes in the absence of dislocation.

From the misfit energy, two interesting properties can be extracted. The first one is the minimum of the misfit energy which is the inelastic part of the energy cost to create a dislocation. Its amplitude is the Peierls energy barrier, that is related to the dislocation motion. Also from the misfit energy, the stress can be calculated by:

$$\sigma = \frac{1}{b}\frac{dW(u)}{du} \quad (4)$$

The maximum of the stress is known as Peierls stress or Critical Resolved Shear Stress (CRSS) and represents the minimum stress necessary to move the dislocation. The glide plane with lower CRSS will be the dominant slip plane in the system. Moreover, the ratio between the CRSS for the glide planes is important in order to determine if a given plane can be activated.

By solving the PN model using as input the GSF, the properties of the dislocations in MgO (misfit energies, Peierls barriers and CRSS) have been determined and are shown in Table 2. We can compare the different properties of the planar dislocations in MgO and quantitatively connect them to the relative importance between the slip planes studied.

Our results indicate that the inelastic core energy of the planar dislocation in $\{110\}(1\bar{1}0)$ is higher that for the other two slip planes. However, even more interesting, the Peierls energy for this plane is one order of magnitude lower than the other ones, which are similar between them. As mentioned before, the Peierls energy is the energy barrier for the dislocation motion. In addition to this, the Peierls stress of $\{110\}(1\bar{1}0)$ is much lower than $\{100\}(011)$ and $\{111\}(1\bar{1}0)$. All together our results confirm that $\{110\}(1\bar{1}0)$ is the dominant slip plane in MgO at low temperature and pressure. The agreement between the calculated results and the experimental data [2,9] is very good. This shows that our procedure and models provide a *quantitative* determination of the dislocation properties in crystalline MgO.

4. Conclusion

Combining the generalized stacking fault energies (GSF) with the Peirls-Nabarro model we have characterized the dislocation properties in the ionic crystal MgO. We have observed that the full dislocation $\{110\}(1\bar{1}0)$ dissociates in partials. The agreement with experimental data for the Critical Resolved Shear Stress is very good. The results also confirm the experimental finding that $\{110\}(1\bar{1}0)$ is the dominant slip plane in MgO at low temperature and pressure. This methodology within the interatomic model used shows that it is possible to have a quantitative description of dislocations in ionic systems. Further investigations on the effects of finite temperature and pressure, as well the geophysical consequences will be reported in elsewhere.

References

[1] R.E. Cohen and J. Weitz, High Pressure-Temperature Research: Properties of Earth and Planetary Minerals, edited by M. H. Manghnani and T. Yagi (AGU. Washington, D.C. 1998), p. 185.

[2] S. Merkel et al., J. Geophys. Res., 107, 2271 (2002).

[3] S. Merkel, Nature, 428, 812, (2004).

[4] B. Joos, Q. Ren and M.S. Duesbery, Phys. Rev. B 50, 5566 (1994).

[5] Y.-M. Juan and E. Kaxiras, Phil. Mag. A 74, 1367 (1996).

[6] M. S. Duesbery and G. Y. Richardson, Crit. Rev. Sol. State and Mat. Sci. 17 1 (1991).

[7] C. R. Miranda and S. Scandolo, to be published.

[8] P. Tangney and S. Scandolo, J. Chem. Phys. 119, 9673 (2003).

[9] C. Meade and R. Jeanloz,J. Geophys. Res., 93, 3261 (1988).

Table 1
Parameters characterizing dislocations in MgO.The Burgers vector (b), the elastic parameter (K), the widths (ζ) of the calculated dislocation profiles, the maximum values of the GSF surface (γ_{max}) and restoring forces (τ_{max}) for the main slip systems in MgO.

	Slip systems		
	$\{110\}(1\bar{1}0)$	$\{100\}(011)$	$\{111\}(1\bar{1}0)$
b ($\AA$)	2.978	2.978	2.978
K($eV/\AA^3$)	0.980	0.918	1.107
ζ(Å)	2.002	1.305	0.671
γ_{max}(eV/Å^2)	0.071	0.143	0.143
τ_{max}(eV/Å^3)	0.092	0.156	0.153

Table 2
Properties of dislocations in MgO obtained from the Peierls-Nabarro model. Misfit energy (W_m), Peierls energy (W_P) and Critical Resolved Shear Stress (CRSS) calculated and experimental data (EXPT) for the main slip planes in MgO. Experimental data were taken from references [2,9].

	Slip systems		
	$\{110\}(1\bar{1}0)$	$\{100\}(011)$	$\{111\}(1\bar{1}0)$
W$_m(eV)$	1.414	0.276	0.968
W$_P(eV)$	0.0012	0.062	0.047
CRSS(GPa)	0.066	3.54	2.76
CRSS$_{EXPT}(GPa)$	0.06	> 1.1	2.6

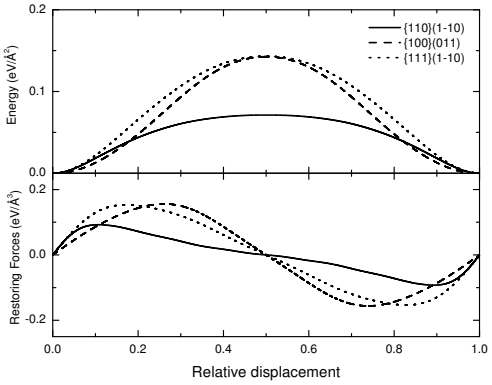

Fig. 1. Stacking fault energy profile (a) and restoring forces (b) for the main slip planes in MgO.

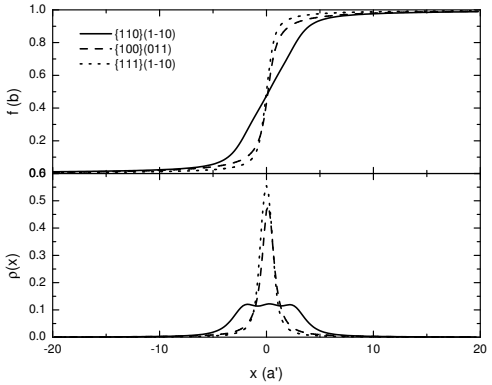

Fig. 2. Dislocation profile, $f_b(x)$ (a) and dislocation density (ρ_b) for the main slip planes of MgO