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Influence of iron on the plastic properties of MgSiO3 post-perovskite: a first-principle study.

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The D” layer is one of the most enigmatic part of the Earth s interior and has major implications for its dynamics. This layer is characterized by a strong and inhomogeneous seismic anisotropy. This latter could be produced by combining the single-crystal elastic anisotropy and crystal preferred orientation (CPO) of (Mg,Fe)SiO{sub}3{/sub} post-perovskite phase. Some experiments have been done on the plasticity of poor-Fe-bearing and pure MgSiO{sub}3{/sub} post-perovskite and lead to textures of deformation dominated by the (100) and (110) slip planes (Merkel et al., 2007) and by the (001) slip plane (Miyagi et al., 2010). On the other hand, theoretical calculations on the dislocations mobility on pure MgSiO{sub}3{/sub} (Carrez et al., 2007; Metsue et al., 2009) suggested a texture dominated by the (010) slip plane. These results cannot explain the seismic observations in the whole D” layer. Consequently, in order to understand the seismic anisotropy of the whole D” layer, one should determined the effects of incorporated elements, such as iron, on the plastic properties of the post-perovskite phase.

In this study, we present the results of an atomic-scale computational study on the plastic shear of pure and Fe-bearing MgSiO{sub}3{/sub} post-perovskite at 120 GPa. We determine the response of 4 potential slip planes, (100), (010), (001) and (110), under a plastic shear through the calculation of the Generalized Stacking Faults (GSF) energies. The values of the GSF energy are obtained by shearing half of an infinite crystal over the other half for every slip plane, similarly to our previous studies for the post-perovskite phase (Carrez et al., 2007; Metsue et al., 2009). The calculation of the GSF energies provides also an estimation of the ideal shear stress (ISS); the maximum resolved shear stress that a perfect crystal can suffer without plastically deforming (Paxton et al., 1991). The GSF energies are determined with ab initio calculations based on the internally consistent LDA+U technique (Tsuchiya et al., 2006) to describe accurately the local interactions between the d-states in Fe. The U parameter is optimized at 120 GPa by using the linear response theory based on the constrained total energy variational principle (Cococcioni and de Gironcoli, 2005, Phys. Rev. B). In this study, Fe is incorporated as substitutional single-point defects close to the glide plane. Iron is treated with different oxidation states (+2 or +3) and different spin states (low or high). As a main result, we show that the incorporation of iron in the post-perovskite phase leads to a decrease of the ideal shear stress for all slip systems. In addition, the slip systems that exhibit the lowest ISS are the same in pure and Fe-bearing MgSiO{sub}3{/sub} post-perovskite.

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Keywords: post-perovskite, first-principle calculations, Stacking fault