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Predictions of the shear response of Fe-bearing MgSiO3 post-perovskite at lowermost mantle pressures
Predictions of the shear response of Fe-bearing MgSiO3 post-perovskite at lowermost mantle pressures

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Observation of seismic data put in forth evidence of a spatial anisotropy in the seismic wave velocities in the D"layer, the lowermost part of the mantle. (Mg,Fe)SiO_3 post-perovskite (PPv) is thought to be the most abundant phase in this part of the mantle.This mineral exhibits a strong elastic anisotropy and may contribute significantly to the seismic anisotropy in the D" layer. However, the seismic anisotropy cannot be expressed at the rock scale if the orientations of the grains are distributed randomly. Consequently, the formation of lattice preferred orientations with an anisotropic mechanism of plasticity, such as dislocation creep, can cause the seismic anisotropy in the D" layer. Some experiments have been done on the plasticity of pure and Fe-bearing $MgSiO_3$ post-perovskite and lead to textures of deformation dominated by the (100) and (110) slip planes (Merkel et al., 2007) or by the (001) slip plane (Miyagi et al., 2010). On the other hand, theoretical calculations on the dislocations mobility on pure $MgSiO_3$ (Carrez et al., 2007; Metsue et al., 2009) suggested a texture dominated by the (010) slip plane. A first step to understanding the mechanisms of plasticity and, therefore, the shear wave splitting occurring in the deep Earth is to test the response of the PPv phase to a plastic shear in a geophysical relevant composition.

In this study, we present new results from first-principles calculations on the shear response of pure and ferrous Fe-bearing $MgSiO_3$ PPv. The originality of this work is the use of internally consistent LSDA+U formalism to accurately describe the local interactions between the d-states of Fe. About 8% of Fe^{2+} is incorporated in the high spin and low spin states, as a Mg substitution defect, to test if a spin transition could be induced by shearing mechanisms, even several studies report that Fe^{2+} is in the high spin in the D" layer pressure range (Stackhouse et al., 2006; Metsue and Tsuchiya, 2011). The response of the PPv to a plastic shear is investigated at 120 GPa through the calculations of the Generalized Stacking Faults (GSF) energy in pure and Fe-bearing systems for 10 potential $<uvw>\{hkl\}$ slip systems, since these latter are not well constrained for the PPv phase. The GSF energies are obtained by shearing homogeneously half of an infinite crystal over the other half for every slip system and give the value of the ideal shear stress (ISS), which can be defined as the theoretical elastic limit of the crystal. The [100](001) slip system in pure and Fe-bearing phases exhibits the lowest ISS and may play an important role in the plastic deformation of the PPv phase. The activation of this slip system is compatible with the observed shear wave splitting $V_{SH}>V_{SV}$. We show that incorporation of Fe decreases the GSF energy and the ISS of all slip systems. In particular, the decreasing of the energy of stable stacking faults indicates that Fe tends to be adsorbed in the stacking faults, which increases the width of the defect and could have some implications on deformation mechanisms. Finally, we discuss the plastic anisotropy of pure and Fe-bearing phases from the values of the ISS and the orientation of applied tensile stress. Our results suggest that the incorporation of ferrous Fe in the PPv phase has a limited effect on its plastic anisotropy, and, therefore, on the deformation texture.

キーワード: MgSiO3 post-perovskite, stacking faults, deformation mechanisms
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