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Anisotropic plasticity of $MgSiO_3$ post-perovskite from atomic scale modeling

Alexandra Goryaeva, Philippe Carrez, and Patrick Cordier
UMET, Université Lille1, Villeneuve d'Ascq, France (alexandra.goryaeva@ed.univ-lille1.fr)

In contrast to the lower mantle, the D′′ layer exhibits significant seismic anisotropy both at the global and local scale [1]. Located right above the CMB, the D" represents a very complex region and the causes of its pronounced anisotropy are still debated (CPO, oriented inclusions, layering, thermo-chemical heterogeneities etc). Among them, contribution of the post-perovskite rheology is commonly considered to be substantial. However, for this high-pressure phase, information about mechanical properties, probable slip systems, dislocations and their behavior under stress are still extremely challenging to obtain directly from experiments [3, 4]. Thus, we propose employing full atomistic modeling (based on the pairwise potential previously derived by [2]) to access the ability of $MgSiO_3$ post-perovskite to deform by dislocation glide at 120 GPa.

Lattice friction opposed to the dislocation glide in $MgSiO_3$ post-perovskite is shown to be highly anisotropic. Thus, remarkably low values of Peierls stress (1 GPa) are found for the glide of [100] screw dislocations in (010), while glide in (001) requires almost 18 times larger stress values. In general, (010) plane is characterized by the lowest lattice friction which suggests (010) deformation textures. Comparison of our results with previous study of $MgSiO_3$ perovskite (bridgmanite) [5], based on similar simulation approach, clearly shows that monotonous increase in Peierls stress of bridgmanite will be followed by a dramatic drop after the phase transition to the post-perovskite phase, which consequently suggests the D′′ located at the CMB to be weaker than the overlying mantle. In addition to that, the observed evolution of CRSS with temperature clearly demonstrates that post-perovskite deforms in the athermal regime which backs up it to be a very weak phase and indicates its deformation by dislocation glide in contrast to high-lattice friction perovskite (bridgmanite) phase deformed by climb only.

References
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