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Deformation, crystal preferred orientations, and seismic anisotropy in the Earth’s D" layer

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We use a forward multiscale model that couples atomistic modeling of intracrystalline plasticity mechanisms (dislocation glide ± twinning) in $MgSiO_3$ post-perovskite (PPv) and periclase (MgO) at lower mantle pressures and temperatures to polycrystal plasticity simulations to predict crystal preferred orientations (CPO) development and seismic anisotropy in D". We model the CPO evolution in aggregates of 70% PPv and 30% MgO submitted to simple shear, axial shortening, and along corner-flow streamlines, which simulate the transition between a downwelling and flow parallel to the core-mantle boundary (CMB) within D" or between CMB-parallel flow and upwelling at the borders of the African or the Pacific large low shear wave velocity provinces (LLSVP). Axial shortening results in alignment of PPv [010] axes with the shortening direction. Simple shear produces PPv CPO with a monoclinic symmetry that rapidly rotates towards parallelism between the dominant [100](010) slip system and the macroscopic shear. Development of PPv and MgO CPO results in seismic anisotropy in D": fast P-waves propagate and fast S-waves are polarized mainly parallel to the shear direction, that is, horizontally for shear parallel to the CMB. ScS and Sdiff delay times depend strongly on the propagation direction (backazimuth). Downwelling flow results in inclined (relatively to the CMB) fast polarizations for Sdiff and ScS waves, with anisotropies varying from null to 5% as a function of the backazimuth. Change in the flow to shear parallel to the CMB produces local weakening of the anisotropy and complex S-wave splitting patterns, with strong variations in fast polarization direction (from nearly parallel to up to 70° to CMB) and birefringence (0-4%) up to 250 km from the corner. Transition from horizontal shear to upwelling produces less weakening of the CPO, because twinning accommodates the change in deformation field; inclined fast polarizations develop in the upwelling path. Models with twinning in PPv explain most observations of seismic anisotropy in D" if the flow departs locally from shearing parallel to the CMB. Heterogeneity of the flow at scales < 1000 km is needed to comply with observation of S-waves polarization anisotropy typically $\leq 2\%$ in D" and with discrepancy in SKS and SKKS birrefringence data at single stations.