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Atomistic study on the generation and gliding properties of pyramidal dislocations in magnesium HIDEO KABURAKI, MITSUHIRO ITAKURA, MASATAKE YAMAGUCHI, Japan Atomic Energy Agency — Plastic deformation of magnesium and its alloys is attracting great interest as one of the candidate materials for energy-conserving lightweight structural metals. The generation of non-basal pyramidal dislocations near the c-axis direction is the key to enhancing plasticity in these highly anisotropic hcp magnesium materials. However, the fundamental understanding of the generation and gliding properties of pyramidal dislocations is still not clear because of the large Burgers vector. Using the molecular dynamics method, we have successfully generated $< c + a >$ type I and II screw dislocations from the crack set in the perfect magnesium crystal by applying the shear stress. Visualization of these dislocations is important because the core structures are complex and largely extended. Comparing the results by first-principles calculations, we have found that the core of the type I screw dislocation is smoothly extended while that of the type II screw dislocation has a corrugated structure. We also found that both dislocations can easily cross-slip to other slip planes. In particular, it is observed that the core of the gliding pyramidal type I screw dislocation cross-slips to other slip planes. The detailed processes of cross-slip are elucidated in the presentation.

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