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Atomistic Mechanism of Plastic Deformation During Nanoindentation of Titanium Aluminide JOSE PEDRO RINO, Universidade Federal de Sao Carlos, CLAUDIO J. DASILVA, Pontifiia Universidade Catolica de Goias —
The mechanisms governing defect nucleation in solids are of great interest in all material science branches. Atomistic computer simulations such as Molecular Dynamics (MD), has been providing more understanding of subsurface deformations, bringing out details of atomic structures and dynamics of defects within the material. In the present work we show the first simulation measurements within an atomistic resolution of the mechanical properties of titanium aluminide intermetallic compound (TiAl), which is a promising candidate for high temperature applications with remarkable properties, such as: attractive combination of low density, high melting temperature, high elastic modulus, and strength retention at elevated temperatures, besides its good creep properties. Through calculations of local pressure, local shear stress and spatial rearrangements of atoms beneath the indenter, it was possible to quantify the indentation damage on the structure. We have founded that prismatic dislocations mediate the emission and interaction of dislocations and the activated slip planes are associated with the Thompson tetrahedron. Furthermore, using the load-penetration depth response, we were able to estimate the elastic modulus and the hardness of the TiAl alloy. All our findings are in well agreement with experimental results.

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