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MOLECULAR DYNAMICS SIMULATION OF STRESS INDUCED GRAIN BOUNDARY MIGRATION DURING NANOINDENTATION EXPERIMENTS

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Molecular dynamics (MD) simulation was performed to study the stress induced grain boundary migration caused by the interaction of dislocations with a grain boundary. The simulation was carried out in a Ni block (295020 atoms) with a $\sum = 5$ (210) grain boundary and an embedded atom potential for Ni was used for the MD calculation. Stress was provided by indenting a diamond indenter and the interaction between Ni surface and diamond indenter was assumed to have a fully repulsive force to emulate a traction free surface. Results showed that the indentation nucleated perfect dislocations and the dislocations produced stacking faults in the form of a parallelepiped tube. The parallelepiped tube consisted of two pairs of parallel dislocations with Shockley partials and was produced successively during the penetration of the indenter. The dislocations propagated along the parallelepiped slip planes and fully merged onto the $\sum = 5$ (210) grain boundary without emitting a dislocation on the other grain. The interaction of the dislocations with the grain boundary induced the migration of the grain boundary plane in the direction normal to the boundary plane and the migration continued as long as the dislocations merged onto the grain boundary plane. The detailed mechanism of the conservative motion of atoms at the grain boundary was associated with the geometric feature of the $\sum = 5$ (210) grain boundary.