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Dislocation Mobility and Cross-slip in Copper - A Molecular Dynamics Study DAN MORDEHAI, School of Physics and Astronomy, The Raymond and Beverly Sackler Faculty of Exact Sciences Tel Aviv University, Tel Aviv 69978, Israel, GUY MAKOV, Department of Physics, NRCN, P.O. Box 9001, Be'er Sheva, Israel, ITZHAK KELSON, School of Physics and Astronomy, The Faculty of Exact Sciences Tel Aviv University, Tel Aviv 69978, Israel — The dynamic properties of dislocations constitute one of the basic building blocks of any theory of plasticity. Experiments are not able yet to follow in detail the microscopic dynamic properties of the dislocation, such as dislocation motion or cross-slip, while atomistic simulations may serve as a powerful tool. Using molecular dynamics (MD) methods the dynamic properties of screw dislocations had been studied in detail for Cu, both as a function of the temperature and the applied stress. Upon applying a glide stress on the dislocation a transition from inertial to viscous motion with a stress dependent terminal velocity is observed. The experimentally observed stress dependence of the terminal velocity is reproduced quantitatively by our results [1]. Upon applying a narrowing stress on the dislocation, in a dislocation dipole structure, cross-slip occurred and the cross-slip rate in the calculations was found to be temperature and stress dependent, as expected. From these calculations the cross-slip mechanism was identified and the activation energy and volume was calculated. [1] D. Mordehai et. al. Phys. Rev. B, 67 024112 (2003)

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