Atomistic simulations of dynamics of Grain Boundary motion coupled to shear deformation

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Abstract

Molecular Dynamics (MD) simulations of shear coupled motion of [001] Grain Boundaries (Gbs) in Ni have been performed. Atomic interactions were modeled by an Embedded-Atom method potential. An external shear stress is applied at a constant velocity. GB response under an external stress is characterized by a stick-slip behaviour, found in many atomic friction processes. GB moves in its normal direction accompanied by a rigid translation of the adjacent grains. When a critical stress is reached, the GB jumps to a neighbor position and the stress drops. The time dependece of the stress has a saw-tooth shape. In the absence of temperature and within a low temperatures range, the stick-slip behaviour works. As temperature increases, thermal activated mechanisms help in overcome the energy barrier, so the GB jumps before the critical stress is reached. In this regime, the saw-tooth shape is not as clear as at lower temperatures was, coupled motion can be eventually destroyed. At high temperatures, sliding events can occur, now GB motion is described as a Brownian motion. This phenomenom has been analysed using geometrical approaches, allowing a comparison with the simulation results. Atomistic simulations provide a further insight of plastic deformation of nano-crystalline Ni.

References

[1] J.W. Cahn et al. Acta Mater. 54 (4953-4975), 2006
[2] V.A. Ivanov et al. Phys. Rev. B. 78 (064106) 2008

Figures

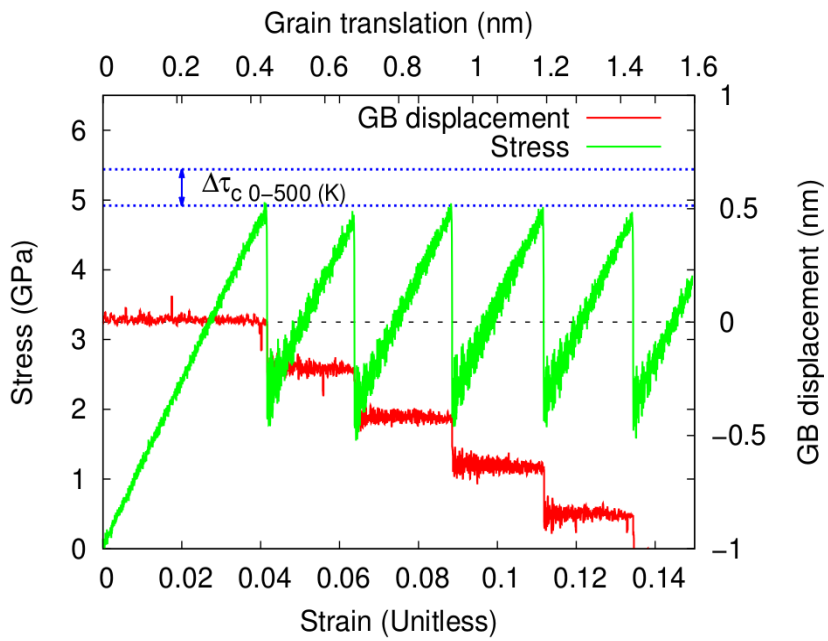

Figure 1. Stress-strain and GB displacement during coupled motion of the Σ17(410)[001] at 500 K. The shear rate is 1 m/s. Dashed blue lines show the decreased of the critical stress with temperature, compared to critical stress at 0 K.

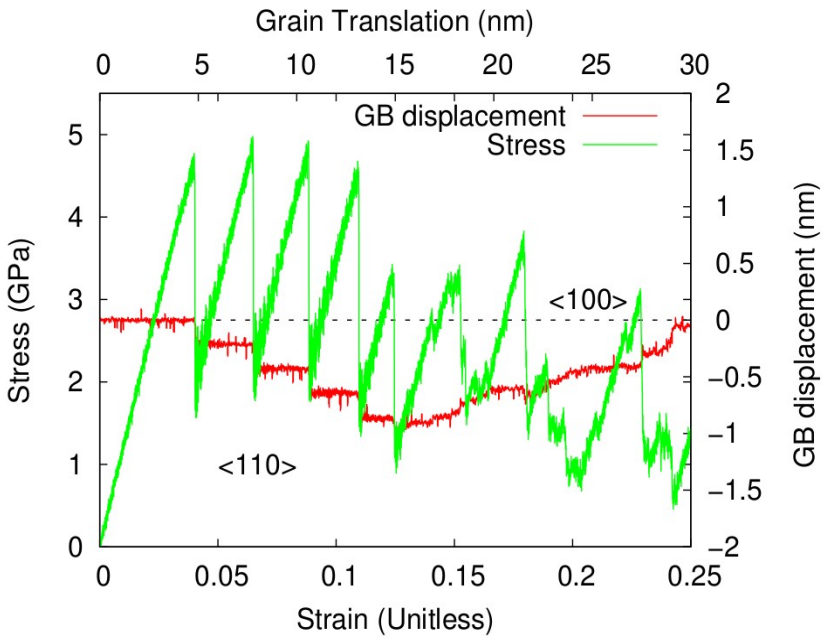

Figure 2. Dual behaviour of Σ17(410)[001] at 600 K. The mode transition between <110> to <100> occurs after 1.7 ns. Stick-slip behaviour is observed in the first stage, after the GB motion is random walk.

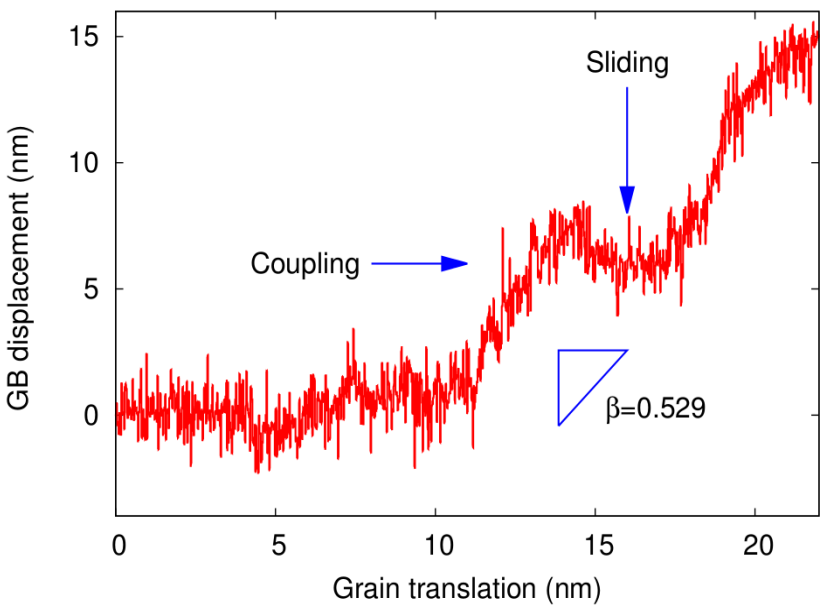

Figure 3. Coupled GB motion interrupted by sliding events at 800 K for Σ17(410)[001]. The imposed shear rate is 1 m/s. Arrows near horizontal region indicate sliding events, alternated with coupled motion of the GB.