# The effect of temperature and stress on creep behaviour of ultrafine grained nanocrystalline Ni-3 at% Zr alloy

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In this paper, molecular dynamics (MD) simulation based study of creep behavior for nanocrystalline (NC) Ni-3 at% Zr alloy having grain size ~ 6 nm has been performed using embedded atom method (EAM) potential to study the influence of variation of temperature (1220-1450 K) as well as change in stress (0.5-1.5 GPa) on creep behavior. All the simulated creep curves for this ultra-fine grained NC Ni-Zr alloy has extensive tertiary creep regime. Primary creep regime is very short and steady state creep part is almost absent. The effect of temperatures and stress is prominent on the nature of the simulated creep curves and corresponding atomic configurations. Additionally, mean square displacement calculation has been performed at 1220 K, 1250 K, 1350 K, and 1450 K temperatures to correlate the activation energy of atomic diffusion and creep. The activation energy of creep process found to be less compared to activation energies of self-diffusion for Ni and Zr in NC Ni-3 at% Zr alloy. Formation of martensite is identified during creep process by common neighbour analysis. Presence of dislocations is observed only in primary regime of creep curve up till 20 ps, as evident from calculated dislocation density through MD simulations. Coble creep is found to be main operative mechanism for creep deformation of ultrafine grained NC Ni-3 at% Zr alloy. More in: **Metals and Materials International (2017). DOI: 10.1007/s12540-017-6144-8**