Microscopic theory of structures and properties of segregated grain boundaries in metals and ceramics

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Grain boundaries in metals and in ceramics, due to local structural deviations from the interior of grains, control the mechanical deformation, fracture and creep, the thermodynamic phase equilibria and transformations, and the kinetics of diffusion, electron and ion conductance of polycrystalline microstructures. For a fundamental understanding − as a prerequisite for an improved design of materials − the energetic stability, atomistic structure and electronic bonding at model twin boundaries, with selected grain misorientations and interface terminations, are investigated by ab−initio density functional theory, with norm−conserving pseudopotentials and a mixed basis of plane waves and local orbitals. The results are compared quantitatively with experimental observations by high−resolution and analytical transmission electron microscopy, and with atomistic simulations based on empirical interatomic potentials. In this lecture, influences of segregated foreign atoms on the structures and energetics of grain boundaries are discussed by considering two cases: (1) symmetrical tilt grain boundaries in Nb and Mo crystals with segregated interstitial B, C, N and O atoms; (2) twin boundaries in Corundum with substitutional cation impurities.