東京大学大学院工学系研究科　総合研究機構

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Crystal Interface Lab. Seminar Series

Theoretical study of dislocations in perovskite oxides

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Perovskite oxides such as barium-strontium titanate, lead zirconate-titanate, or potassium-sodium niobate are technologically important and scientifically exciting materials. Many perovskites are ferroelectric and possess high dielectric constants, which make them attractive for modern microelectronic applications. A successful implementation however requires not only information about the intrinsic functional properties but also a thorough understanding of crystal defects that influence the functionality as well as the mechanical and structural stability of such components.

In the present work we investigate the properties of dislocations in perovskite materials by means of atomistic simulations, using both accurate first-principles calculations (density functional theory) and computationally efficient atomistic simulations with classical interatomic potentials [1,2]. In paraelectric strontium titanate the structures of dislocation cores are analyzed and compared to high-resolution transmission electron microscopy observations. The calculated Peierls energies and stresses for these dislocations under different applied loads give insight into their mobilities and are related to the macroscopic mechanical behavior. In ferroelectric perovskites we study the motion of a domain wall under an applied electric field, and the pinning by a dislocation at the atomic scale.

[1] P. Hirel, P.Marton, M. Mrovec , C. Elsaesser, Acta Mater. **58** (2010) 6072.

[2] P. Hirel, M. Mrovec , C. Elsaesser, Acta Mater. **60** (2012) 329.

Main meeting room at Institute of Engineering Innovation, UT

工学部総合研究機構 9号館1階　大会議室

2013, July 26th (Fri.) 10:00~11:30