Surface and Quantum-Confinement Effects in Ultrathin MoSi2 films

LIANG-FENG HUANG, JAMES RONDINELLI, Northwestern University — Mo-Si-based alloys are promising structural materials for ultrahigh-temperature applications owing to their excellent mechanical strength at elevated temperature. Among the Mo-Si alloys, MoSi2 exhibits outstanding oxidation resistance as a result of native SiO2 scale formation. In this work, using density-functional theory calculations, we propose the alternative novel usage of MoSi2 for nanoelectronics. The cleavage of MoSi2 nanofilms from the layered bulk requires low energy because of the preserved chemical stoichiometry, indicating their facile synthesis in experiment. We explore the surface and quantum-confinement effects by investigating the thickness-dependent structure, stability, and electronic structure of MoSi2 nanofilms, where high carrier concentrations have also been observed. The possible applications of MoSi2 nanofilms as robust metallic substrates, electrodes, and in other nanodevices are discussed. In addition, we also discuss the effect of surface-induced metallicity on Raman spectra of MoSi2, which are frequently used to characterize MoSi2 samples.

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