Abstract Submitted
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N vacancy, self-interstitial diffusion, and Frenkel-pair formation/dissociation in TiN studied by *ab-initio* and classical molecular dynamics[1] DAVIDE G. SANGIOVANNI, BJÖRN ALLING, LARS HULTMAN, IGOR A. ABRIKOSOV, Department of Physics (IFM), Linköping University, Sweden — We use *ab-initio* and classical molecular dynamics (AIMD, CMD) to simulate diffusion of N vacancy and N self-interstitial point-defects in B1 TiN. The physical properties of TiN, important material system for thin film and coatings applications, are largely dictated by concentration and mobility of point defects. We determine N dilute-point-defect diffusion pathways, activation energies, attempt frequencies, and diffusion coefficients as a function of temperature. In addition, MD simulations reveal an unanticipated atomistic process, which controls the spontaneous formation of N-self-interstitial/N-vacancy pairs (Frenkel pairs) in defect-free TiN. This entails that a N lattice atom leaves its bulk position and bonds to a neighboring N lattice atom. In most cases, Frenkel-pair N^I and N^V recombine within a fraction of ns; 50% of these processes result in the exchange of two nitrogen lattice atoms. Occasionally, however, Frenkel-pair N-interstitial atoms permanently escape from the anion vacancy site, thus producing unpaired N^I and N^V point defects.

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