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Particle Impact Induced Point Defect Structure of Titanium Nitride

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Physical vapor deposition (PVD) of titanium nitride (TiN) thin films in case of highly ionized discharges (e.g., HPPMS, cathodic arc) are inherently dependent on particle bombardment at the respective surface site (atop Ti, atop N, Ti-N bridge). In particular, the redistribution of the kinetic energy of the impinging titanium particles (i.e., 100 eV and onward at the target) and the implied structural changes at the atomic scale need to be understood, both qualitatively as well as quantitatively. In the literature fundamental TiN surface and large-scale film growth dynamics have been investigated extensively by D. Sangiovanni and coworkers for low energetic particles [1], whereas a supplementary study of small-scale growth processes has been published as well [2]. A complementary analysis of sputtering by highly energetic ion bombardment has not been reported yet. In this study, a more unified perspective is attained with the aim to cover the complete energy range from growth to sputtering conditions. Hence, for a wide range of kinetic energies deposited at the surface sites (specifically, from 20 to 200 eV) the collisional generation, the evolution, and the relaxation of point defects are investigated. A twofold simulation approach is pursued: Classical molecular dynamics (MD) simulations of the particle impingement on TiN(001) are compared with the outcome of ab initio MD computations. The latter are based on effective thermal spike simulations for which the generation of Frenkel pairs is taken to model the impact of energetic ions (i.e., for energies $\varepsilon > 45$ eV) [3,4]. Together, the development of the titanium nitride point defect structure induced by energetic particle bombardment is discussed in terms of changes in the potential energy surface.

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