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The effect of hydrogen content on intrinsic stress in nanocrystalline diamond (NCD) coatings HAIBO GUO, University of South Carolina, YUE QI, XINGCHENG XIAO, General Motors R&D, ABHISHEK KOTHARI, BRIAN W. SHELDON, Brown University, MATERIALS AND PROCESSES LAB, GENERAL MOTORS R&D COLLABORATION, UNIVERSITY OF SOUTH CAROLINA COLLABORATION, BROWN UNIVERSITY COLLABORATION — The stress control is critical to ensure the reliability of nanocrystalline diamond (NCD) coatings. We found the intrinsic stress in NCD is tensile at deposition temperature above 700°C. Decreasing the deposition temperature decreases this tensile stress, and eventually leads to compressive stresses. The stress evolution appears to be largely dictated by grain boundary formation and hydrogen incorporation, which involves absorption, desorption, and recombination kinetics on diamond surfaces. The competition between these reactions indicates that the hydrogen coverage at interfaces should increase with decreasing growth temperature. This is consistent with Raman spectra and elastic recoil detection. To understand hydrogen effects, density functional theory (DFT) is used to model the coalescence of two diamond grains that approach each other to form a grain boundary. The two surfaces exhibit attractive forces when hydrogen coverage is less than 75%, and repulsive forces when all the surface bonds are hydrogen terminated (100% hydrogen coverage). In this way, differences in the hydrogen coverage can explain the observed transition from tensile to compressive intrinsic stress as the growth temperature decreases.

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