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Ab Initio Based 2D Continuum Mechanics – Sensitivity Prediction for Contact Resonance Atomic Force Microscopy Based Structure Fingerprints QING TU, BJÖRN LANGE, MEMS Department, Duke University, Durham, NC 27708, J. MARCELO J. LOPES, Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin, Germany, STEFAN ZAUSCHER, VOLKER BLUM, MEMS Department, Duke University, Durham, NC 27708 — Contact resonance AFM is demonstrated as a powerful tool for mapping differences in the mechanical properties of 2D materials and heterostructures, permitting to resolve surface and subsurface structural differences of different domains. Measured contact resonance frequencies are related to the contact stiffness of the combined tip-sample system. Based on first principles predicted elastic properties and a continuum approach to model the mechanical impedance, we find contact stiffness ratios between different domains of few-layer graphene on 3C-SiC(111) in excellent agreement with experiment. We next demonstrate that the approach is able to quantitatively resolve differences between other 2D materials domains, e.g., for h-BN, MoS_2 and MoO_3 on graphene on SiC. We show that the combined effect of several materials parameters, especially the in-plane elastic properties and the layer thickness, determines the contact stiffness, therefore boosting the sensitivity even if the out-of-plane elastic properties are similar.

Björn Lange
MEMS Department, Duke University, Durham, NC 27708

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