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Molecular Dynamics Simulations of Surface Acoustic Waves on Patterned Layered Nanostructures[1] MATTEO BJORNSSON, AINE CONNOLLY, SUSHANT MAHAT, BRYAN RACHMILOWITZ, BRIAN DALY, Vassar College, GEORGE ANTONELLI, Antonelli Research & Technology LLC, ALAN MYERS, KANWAL SINGH, HIU-JAE YOO, SEAN KING, Intel Corporation — We report coarse-grained molecular dynamics (MD) simulations of surface acoustic waves on patterned layered nanostructures. The simulations were designed for comparison with samples consisting of the following patterned film stack: 25 nm physically vapor deposited TiN / 180 nm porous PECVD-grown a-SiOC:H / 12 nm non-porous PECVD-grown a-SiOC:H etch-stop / 100 nm CVD-grown a-SiO_2 / Si (100) substrate. The TiN film was etched with lines of rectangular cross-section with pitch = 168 to 420 nm. Ultrafast optical experiments on these samples have detected high frequency surface waves in the range of 10's of GHz. The MD simulation demonstrates the presence of strongly excited modes at frequencies that closely match those found in the experiments. Moreover, the simulation predicts that the type of surface wave mode detected should change depending on the pitch. For larger pitch, Rayleigh-like waves are predicted, but for smaller pitch, Sezawa waves (surface waves with properties similar to free plate modes of the thin films) are predicted. The MD simulation also demonstrates the cutoff wavelength for the Sezawa modes, as is reflected in the experimental results and as is also predicted by isotropic elastic calculations of the surface modes of a thin film on an infinite substrate.

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