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Stress effects on Raman spectroscopy of aSi:H – theory and experiment DAVID A. STRUBBE, ERIC C. JOHLIN, Dept. of Materials Science and Engineering, Massachusetts Institute of Technology, TIMOTHY R. KIRKPATRICK, TONIO BUONASSISI, Dept. of Mechanical Engineering, Massachusetts Institute of Technology, JEFFREY C. GROSSMAN, Dept. of Materials Science and Engineering, Massachusetts Institute of Technology — Raman microscopy has proven to be a very useful technique for inferring stress distributions in materials, since the positions of vibrational peaks are sensitive to local stress. This method has been applied extensively for crystalline silicon, and would be useful for amorphous silicon as well, particularly for studying local stress and composition of nanostructured amorphous/crystalline devices. Toward that goal, we have simulated the Raman spectrum of hydrogenated amorphous silicon with density-functional perturbation theory, using atomistic structures from the WWW algorithm with different stress states. We obtain a spectrum in good agreement with experimental results, and calculate a coefficient for the change in the TO peak position proportional to stress. We then performed Raman experiments on an a-Si:H film deposited on a c-Si wafer, in which stress was applied with a 4-point bending setup, and found a stress coefficient consistent with the simulations, in contrast to inconsistent previous results in the literature. These results can be used to map out local stress distributions, and also relate to thermal expansion and vibrational anharmonicity via the Grüneisen parameter.

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