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Two-Level Systems and Growth-Induced Thermodynamic Metastability in Hot-Wire Deposited Hydrogenated Amorphous Silicon[1]

MANEL MOLINA-RUIZ, HILARY JACKS, FRANCES HELLMAN, Department of Physics, University of California Berkeley, Berkeley, CA 94720, DANIEL QUEEN, Northrop Grumman Corporation, Linthicum, MD 21090, XIAO LIU, Naval Research Laboratory, Washington D.C., 20375, QI WANG, RICHARD CRANDALL, National Renewable Energy Laboratory, Golden, Colorado 80401 — Hydrogenated amorphous silicon (a-Si:H) prepared by hot-wire chemical vapor deposition (HWCVD) shows a large specific heat C_P at low temperature T, despite low values of tunneling level states as measured by internal friction. C_P is significantly larger than the Debye specific heat calculated from the sound velocity, characteristic of glasses with two-level systems (TLS). The as-prepared films have an additional Schottky-like anomaly at low temperature that is associated with metastable hydrogen in the amorphous network. Annealing at 200 C, well below the growth temperature, irreversibly reduces C_P by over an order of magnitude below 12 K, eliminating the Schottky-like anomaly. Based on the linear term in C_P, the TLS density in this annealed state is orders of magnitude larger than expected based on internal friction Q^{-1} measurements, which are unchanged by the anneal. This large TLS density is suggested to result not from a local Si-H excitation, but instead from atomic scale regions best described as Si-H complexes in the a-Si network. Comparison of heat capacity to internal friction suggests that these TLS are decoupled from acoustic excitations.

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