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An Investigation of the Effects of Hydrogen on Local Strain Fields and Structural Disorder-to-Order Transition in Hydrogenated Amorphous Silicon

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Abstract: This study utilizes the fluctuations in the mean silicon-silicon near neighbour distances and local atomic-level stresses to study the chemically-induced disorder-to-order transition in hydrogenated amorphous silicon as a function of hydrogen concentration C_H. The correlation between a suitable stress and structure parameter shows a three-stage structure transition that culminates in the formation of a crystalline phase at high C_H. In the low C_H limit, the structural changes are characterized by a linear response to stress giving a rigidity modulus of 73.43+-15 GPa. In the intermediate and high C_H limits, the stress-structure correlation shows a volume-dependence. At very high hydrogen concentrations, a high rigidity modulus is obtained in good agreement with the rigidity of crystalline silicon. An interpretation of the results in terms of the constraint counting model of the continuous random network suggests that the observed high modulus of rigidity characterizing the crystalline phase is a direct consequence of the reduction in volume fraction due to increased hydrogen bonding.

Key Words: Amorphous silicon, atomic-level stress, defects, topological disorder, local order, strain-fields

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