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Growth and optical properties of embedded silicon nanocrystals[1]

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The optoelectronic properties of nanostructured silicon (nc-Si) are governed by the interplay between the local chemical bonding features and the complex overall atomic structure. Interesting enough, a-Si has a larger optical absorption than the c-Si and, therefore, biphasic a-c silicon systems (i.e. nanocrystallites embedded into an amorphous matrix) are currently under investigation for next-generation photovoltaics. Biphasic systems undergo crystallization upon thermal annealing and, therefore, it is quite difficult to predict theoretically their finite-temperature optoelectronic properties. In this talk I will present our ongoing research on the growth and the optoelectronic properties of textured nanocrystalline silicon, here modeled as a distribution of cylindrical grains embedded into an amorphous matrix. As for the growth, I argue that by large-scale atomistic simulations it is possible to infer a continuum model for the crystallinity evolution upon thermal annealing.[1] In particular, at low crystallinity, it is proved that–consistently with the standard Kolmogorov-Johnson-Mehl-Avrami (KJMA) theory–the a-c phase transformation is dominated by the isolated grain evolution; conversely, at later stages deviations from the KJMA theory are observed, mainly due to atomic-scale features. I also prove that such effects can be included by using an improved phenomenological version of the KJMA theory.[2] As for the finite-temperature optoelectronic properties, I present a divide-and-conquer computational procedure, based on a combination of empirical tight-binding and model-potential molecular dynamics. This procedure is applied to investigate local and average optoelectronic properties of very large nanostructured silicon systems and to predict the variation of the optical absorption upon crystallinity.[3] I show that the optical absorption of a nc-Si sample corresponds to a simple linear combination between c-Si and a-Si phases and it is not affected by electron confinement within grains. Strain effects on combined absorption are discussed as well.

[1] A. Mattoni, L. Colombo, Phys. Rev. Lett. 99, 205501 (2007)
[2] A. Mattoni, L. Colombo, Phys. Rev. B 78, 075408 (2008)
[3] A. Mattoni, L. Colombo, submitted (2008)

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