High sensitivity optical characterization of thin films with embedded Si nanocrystals

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Optical techniques have long been proven to be highly sensitive tools for thin film and nanocrystal characterization. The capability of measuring the change of phase by reflection of polarized light using ellipsometry on a surface or layer structure allows a typical sensitivity of less than one nanometer for the layer thickness and 10^{-3}-10^{-4} for the refractive index. These capabilities together with a spectroscopic use in the photon energy range of the characteristic interband transitions makes the method applicable for an accurate determination of nanocrystal properties especially for Si, but also for wide band gap semiconductors using an extension into the deep UV spectral range. The sensitivity is high, down to the smallest nanocrystal sizes. The requirement for an accurate nanocrystal measurement is a layered form with optical quality interfaces. The thickness, homogeneity and interface qualities of the layers can be measured using conventional and widely used optical models, whereas the properties related to the nanocrystal structure (like the crystallinity, the nanocrystal size or the density of the layer) can be obtained using proper optical models that describe the dispersion of the dielectric function.

In this work two major aspects of optical nanocrystal measurements are discussed. The first one is a survey of the parameterizations of the dielectric function [1, 2] from the effective medium approximation to model dielectric functions (Fig. 1), also in combination. The second one is the use of parameter search algorithms that help to avoid or at least minimize the probability of getting into local minima during the fitting of numerous model parameters. Using oscillator models for the description of the dielectric function the number of fit parameters is relatively high. Not only the parameter search but also the analysis of their correlation is crucial, because it helps to find insensitive parameters, and in turn to couple or fix numerous parameters.

Finally, the dispersion of the dielectric function can be used to assess nanocrystal properties like the crystallinity of the layer, size or density of nanocrystals or density of the layer. Since the imaginary part of the dielectric function measured with high sensitivity is proportional to the joint density of electronic states, the change of the dielectric function is a direct fingerprint of the changes in the band structure, and in turn, the changes of nanocrystal properties. The change of the dielectric function is influenced by two major effects. The first one is the quantum confinement, which causes a blue shift of the band gap with decreasing nanocrystal size. The second one is the broadening of the absorption peaks due to electron scattering at the nanocrystal boundaries, which is an indication of the volume fraction of boundaries.

Combined with the effective medium approximation the volume fraction of nanocrystals can also be determined from the fit using sophisticated optical models.

Acknowledgments

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References

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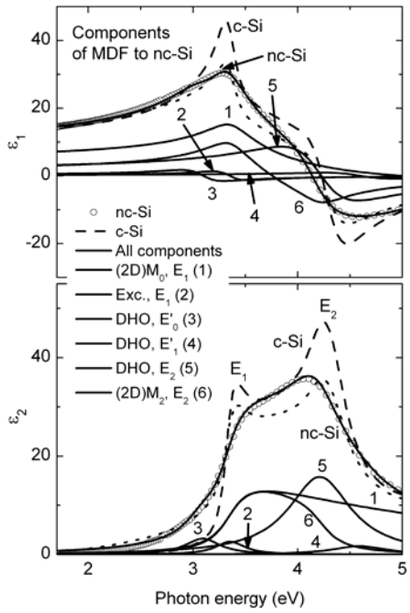

Figure 1: Oscillators of the model dielectric function of S. Adachi (numbered solid lines) fitted to the real (ε_1) and imaginary (ε_2) parts of the reference dielectric function of a fine-grained polycrystalline silicon (nc-Si). The long-dashed line is the single-crystalline silicon (c-Si) reference. The short-dashed line shows the fit using the effective medium approximation with the components of c-Si and a-Si. DHO denotes damped harmonic oscillators, $(2D)M_0$ and $(2D)M_2$ denote two-dimensional critical points.