Numerical modeling of crystal properties: from photonic crystals to monocrystalline silicon.

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The first part of the presentation is devoted to numerical modeling of two-dimensional (2D) photonic crystals optical properties.
Two-dimensional photonic crystals (PhCs) operating in the near-infrared wavelengths are promising candidates for novel integrated optics applications. In the presented work the optical properties of the Bloch modes in 2D photonic crystals have been investigated theoretically using different numerical methods. The plane wave expansion (PWE) method have been formulated in a general form for arbitrary 2D photonic crystals and applied for detailed analysis of the properties of the Bloch modes. The limitations of the PWE method related with the approximation error of the dielectric permittivity discontinuities have been analyzed and an efficient method of suppression of the Gibbs phenomenon has been proposed.
The guided mode expansion method has been used to take into account three-dimensional distribution of the electromagnetic field in the planar photonic crystals and improve the accuracy of the analysis. It has been shown that utilization of this approach provides better agreement with the experimental photonic crystal dispersion curves.
A new method of calculation of the sensitivity of the photonic crystal optical properties to small variations of the photonic crystal parameters has been developed. This method is based on the perturbation theory and allows fast and accurate estimation of the optical properties corrections as a result of a change the parameters of the photonic crystal.
The developed methods proved to be efficient and accurate tools for modeling two-dimensional photonic crystal properties and design of photonic crystal based devices.

The second part of the presentation is devoted to modeling of semiconductor crystal growth from the melt and analysis of the crystal quality.
High quality monocrystalline silicon is the basic semiconductor material for producing integrated circuits. In recent years, crystal homogeneity and microstructure properties have become of high importance, which demands the optimization of the whole technological process. Numerical simulation of crystal growth process has become a fruitful tool for supporting the technology refinement. Using models of heat and mass transfer for a crystal growth system one can study the influence of growth parameters on crystallization conditions and subsequent defect formation in the crystal.
Non-uniform temperature distribution and high temperature gradients near the crystal/melt interface lead to thermal stress, which may be high enough to cause dislocation formation or crystal cracking. An accurate analysis of the stress distribution during the growth process is required to avoid such unacceptable crystal damage. A two-dimensional axisymmetric numerical model for thermoelastic stress calculation has been developed and implemented into the global model of crystal growth process. Calculated distribution of the Von Mises stress provides the key information for the crystal damage prediction.
For silicon crystals produced by the Czochralski technique (CZ) the primary imperfections are point defects: octahedral vacancy aggregates (so-called voids) and particles of amorphous oxygen precipitates SiO_2, which are usually observed in CZ silicon due to a high oxygen concentration in the crystal. In this presentation I describe the developed physical model and numerical approach, which couple the computer efficiency with an accurate description of defect evolution in a growing crystal. The model describes the initial defects incorporation into growing crystal as well as point defects nucleation and subsequent growth during crystal cooling. Utilization of this model provides concentration and size distribution of the point defects in the grown crystal and this information is used for the optimization of the growth condition.