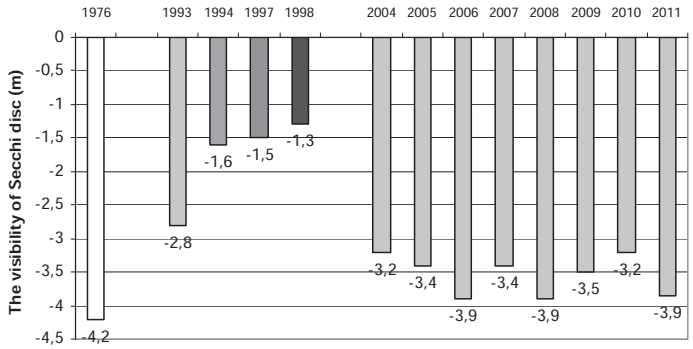

Fig. 4. The Secchi disc visibility in the summer stagnation period, 1976-2011

between 0.8 and 0.9 m during the summer stagnation period. The average values ranged between 2.8 and 1.3 m at that time (Fig. 4).

The visibility of the Secchi disk increased rapidly after the restoration process began. The Secchi disk was normally visible at a depth of 3-4 m for eight years. The maximum visibility of the Secchi disk was observed in July 2012 (7.5 m).

The application of the hypolimnion removal method (Olszewski tube) in Pławniowice Reservoir has therefore been successful, achieving its oligotrophication, i.e. lowering the nutrient content in the ecosystem. Oligotrophication resulted in improvements in water quality, such as a declining internal enrichment process and increased water transparency. The hypolimnion removal apparatus not only enhanced environmental condition of the reservoir, it also constituted a permanent defense mechanism against eutrophication.

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Continuum and atomistic modeling of crystal defects

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The rapid development of experimental techniques such as High Resolution Transmission Electron Microscopy (HRTEM) and tomography has recently allowed for the exploration and examination of material structure in a very wide spectrum of length scales, starting from the picometer through atomistic to the macro scale. In many cases, the nano scale, at which single atoms gather together into more-or-less ordered structures, takes the fundamental role.

The Computational Materials Science Division at the PAS Institute of Fundamental Technological Research specializes in modeling interdisciplinary problems situated on the border of solid mechanics, physics, chemistry, crystallography, and materials science. Special attention is focused on residual

stresses and crystal defects. Such defects significantly affect many physical and chemical properties of real materials, such as semiconductors and nanostructures. Although the main tool of computational materials science lies in computational methods, a crucial role in making progress is played by the theory of constitutive modeling and programing skills. Constitutive modeling is used to solve the problem of how to employ new important data extracted from experimental examination on materials as feedback into research on their characterization and production technology. The method developed at the PAS Institute of Fundamental Technological Research is based on the extraction of tensor and/or scalar fields from experimental images, e.g. lattice distortions or chemical concentrations, and using them in the next step in solving the boundary-value problems by the Finite Element method (FE).

If a structure is more complex than its meshing and the input of tensor fields is of different order into nodes compose more complex problem. As a consequence, prices of good computer programs for preprocessing input data with the FE method often exceed the prices of programs used in the main finite element calculations. Things seem to look no better for preprocessing input data for atomistic and *ab-initio* modeling. For example, there are no numerical methods or programs available using which the atomistic model of a 3D dislocation network with fixed, arbitrary chosen angles between dislocation elements could be preprocessed. By comparison, in preprocessing based on molecular dynamics, the random dislocation networks are generated by the inelastic deformation of initially perfect crystal structures. Figure 2 shows an example of reconstructed atomistic and FE models of a GaN quantum dot nucleated next to an edge dislocation piercing the AlN layer. Such a structure was observed experimentally.

One attempt at multiscale, finite element–atomistic pre-processing of input data is the Visual Editor of Crystal Defects (VECD), developed at the PAS Institute of Fundamental Technological Research (Fig. 1). The computer program gathers together: the processing of experimental data, FE meshing, and a reconstructed atomistic model of crystal defects. Through computer processing of the HRTEM image, a tensor field of lattice distortion can be extracted from computer image processing, and next such a tensor field can be input into a FE mesh. The

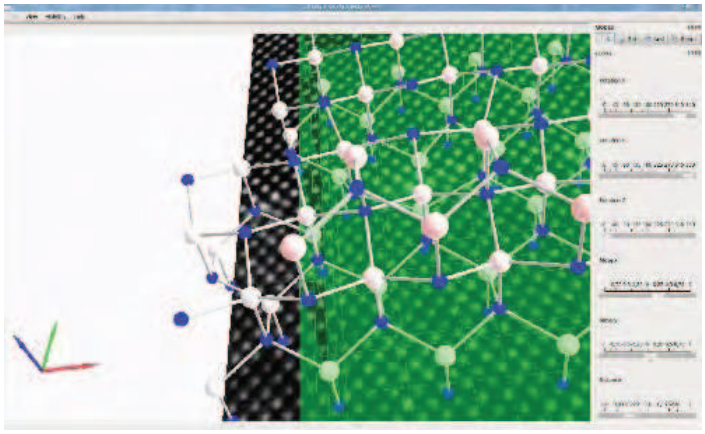

Fig. 1. Visual Editor of Crystal Defects – a program for reconstructing atomistic and finite element models of crystal defects

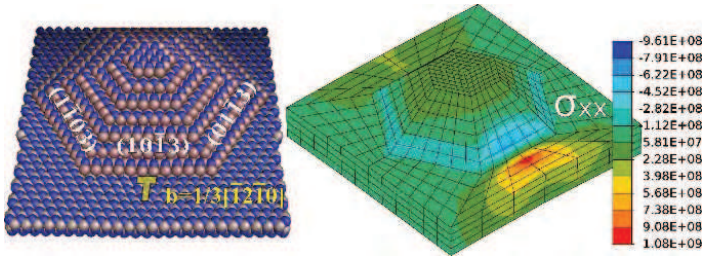

Fig. 2. Atomistic model of GaN quantum dot situated at the border of a threading edge dislocation piercing an A1N layer. The map of resultant residual stresses σ_{xx} has been visualized on the FE mesh

mesh is generated together with an atomistic model of crystal defects visible on the HRTEM image.

At the first step, positions of atoms forming a given dislocation net are reconstructed using a linear theory of dislocation, according to which the displacement of each atom from its initial position X can obtained by the use of the analytical formula $u_j(X)$ corresponding to the formation of the j^{th} elemental dislocation of the dislocation network,

$$u^{o} = \sum_{j=1}^{n} u_j(X)$$

Figure 3, as an example, shows a fragment of a preprocessed atomistic model of a misfit dislocations net formed between copper crystal and sapphire. In subsequent steps, the displacements are iterated to the analytical solution for lattice distortion determined in relation to the so called spatial configuration according to the following scheme:

$$\Delta u^{i+1} = -[1- \beta(X + u^{i})]^{-1} [u^{i} - f(X + u^{i})],$$

where β and f are the analytical functions determined in the linear theory of dislocation, Δu^{i+1} is the

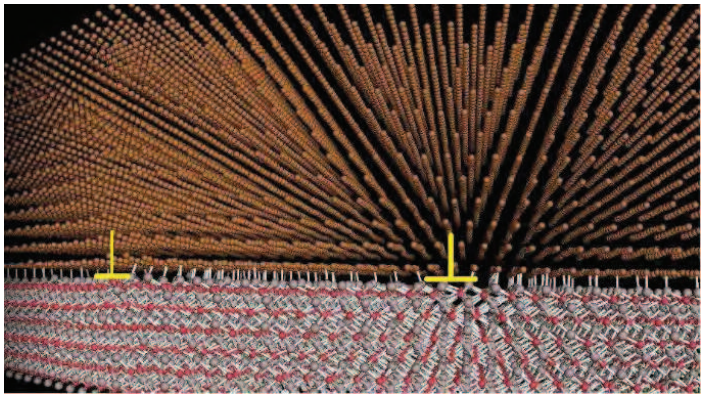

Fig. 3. Atomistic reconstruction of misfit dislocation net in the interfacial zone of Cu/Al_2O_3 heterostructure

shift of a given atom in the i^{th} + 1 iteration. Instead of the aforementioned analytical approach corresponding to solving an implicit equation set, the position of atoms can be fitted directly to positions determined from the HRTEM image and/or to numerical solutions obtained by solving a FE boundary-value problem for chemo-, electro-, and/or -mechanical fields coupled with the residual stresses induced by crystal defects.

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An outline of the mechanics of granular soils

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Sawicki's book (2012) summarizes the results of research on the mechanics of non-cohesive (granular) soils conducted at the PAS Institute of Hydro-Engineering. The author discusses experimental and theoretical investigations of the behaviour of dry and saturated soils before the limit state is reached and under extreme conditions, as well as some theoretical models of soils and the applications of these models for the analysis of important practical problems. His book offers a pioneering perspective on the mechanics of granular soils, unprecedented in the available literature, since it deals with such subjects as the liquefaction of soils and their subsequent resolidification, phenomena associated with the lifting of objects from saturated ground, soil stability, and some elements of seabed dynamics.

Granular soils, such as silts, sands, and gravels, especially when saturated, exhibit certain characteristics that clearly distinguish them from liquids and solids. That is why they are sometimes even referred to as the fifth state of matter. Saturated ground