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Structure characterization of large ZnO crystals from Oława Foundry

Roman Minikayev[1], Jarosław Z. Domagała[1], Elżbieta Dynowska[1], Katarzyna Gas[1], Elżbieta Łusakowska[1], Wojciech Szuszkiewicz[1]*, Józef Cebulski[2], Jakub Grandysa[2], Patrick Baroni[3], and Anthony M.T. Bell[4]

[1] *Institute of Physics, Polish Academy of Sciences, al. Lotnikow 32/46, Warszawa 02-668, Poland*
[2] *Microelectronics and Nanotechnology Center, University of Rzeszów, Rejtana 16a, 35-959 Rzeszów, Poland*
[3] *Laboratoire Leon Brillouin, CEA-CNRS, CE Saclay, Gif-sur-Yvette 91191, France*
[4] *HASYLAB at DESY, Notkestr. 85, Hamburg 22607, Germany*

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e-mail: szusz@ifpan.edu.pl

ZnO is a wide band-gap semiconductor with unique physicochemical properties but development of ZnO-based electronics is strongly limited by the lack of large crystals of high quality suitable for industry as substrates for the homoepitaxy.

The goal of this work is to determine structure properties of unique ZnO crystals obtained as by-product of zinc white production in Oława Foundry. These crystals are about 1 cm wide and about 12 cm long rods with a hexagonal basis. The powder X-ray diffraction measurements confirmed a hexagonal wurtzite structure of the samples (the crystal axis coincides with the wurtzite *c*-axis) and a lack of additional peaks resulting from possible precipitates. Studies with the use of SIMS technique evidenced a presence of Mn and Mg at an impurity level. The analysis of the Bragg peak intensity distribution maps in the reciprocal space showed very homogeneous distribution of defects and small scattering of the mosaic block orientation. The linear expansion coefficients for the *a* and *c* lattice parameters were determined with the use of synchrotron radiation in the temperature range from 15 K to 1100 K at Hasylab.

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Structure of HCC oligomers – SAXS and MD studies

Magdalena Murawska[1], Anders Grubb[2], Martyna Maszota[3], Sylwia Rodziewicz-Motowidło[3], and Maciej Kozak[1*]

[1] *Department of Macromolecular Physics, Faculty of Physics, Adam Mickiewicz University Poznań, Poland*
[2] *Department of Clinical Chemistry, Lund University, Sweden.*
[3] *Department of Chemistry, University of Gdańsk, Poland*

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*e-mail: mkozak@amu.edu.pl

Human cystatin C (HCC) is a small protein (the inhibitor of cysteine proteases) with amyloidogenic properties. Dimerization process of HCC occurs through the three-dimensional exchange of structural domains called as "domain swapping". HCC forms also different oligomeric forms (trimers, tetramers, decamers and other oligomers of higher molecular weights [1-3].

The study presented was aimed at developing low-resolution structure of trimeric form of human cystatin C in solution (stabilized by covalent bonds) and comparing this structure with the structure of HCC trimers calculated by molecular dynamics simulations.

The molecular dynamics simulations were performed using AMBER program package and several structural models of HCC trimers were created. The X-ray scattering data were obtained using synchrotron radiation and SAXS camera (EMBL beam line X33, DORIS storage ring, DESY, Hamburg, Germany; λ= 0.15 nm). Structural models of the human cystatin C trimers in solution were restored by a *ab initio* simulations in program DAMMIN [4]. Low-resolution structure of HCC trimer exhibits the 3-fold axis of symmetry.

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References

[1] R. Janowski, M. Kozak, E. Jankowska, Z. Grzonka, A. Grubb, M. Abrahamson, M. Jaskolski. *Nature Structural Biology* **8** (2001) 316-320.

[2] M. Orlikowska, E. Jankowska, R. Kołodziejczyk, M. Jaskolski, A. Szymańska, *Journal of Structural Biology* **173** (2011) 406-413.

[3] A. Grubb, *Adv. Clin. Chem*. **35** (2000), 63-99.

[4] D.I. Svergun. *Biophys J.***76** (1999) 2879-2886.