In memory of Zinoviy Gurskii

On May 29, 2004 Professor Zinoviy Gurskii, one of the leading Ukrainian experts in the theory of metals and alloys, would be 60. Unfortunately, a heavy illness took away on January 28, 2004 the life of the noted scientist and remarkable person.

Zinoviy Gurskii was born on May 29, 1944 in Lviv. After the secondary school he started in 1961 studies at the Department of Physics of I.Franko Lviv State University. As one of the most talented young Ukrainian students Zinoviy Gurskii spent the last three years of his studies in Moscow and graduated from the M.Lomonosov Moscow State University in 1967. Immediately thereafter he began his research at the A.Baikov Institute of Metallurgy of the Academy of Sciences of USSR in Moscow under the guidance of a well-known expert in solid state theory Professor G.Krasko.

Theory of metals and electronic liquid was among the most urgent issues in the physics in the 60-s of the last century. In the solid state theory a concept of pseudopotential, proposed in 1959 by J.Phillips and L.Kleinman, was very promising in treating the valence states in metals. The Phillips-Kleinman pseudopotential obtained by a transformation of atomic potential due to orthogonalization effects

was much weaker than the atomic potential, which made it suitable for the treatment in the perturbation theory for electron states. Later on, in 1964 V.Heine and I.Abarenkov proposed a method of model pseudopotential, in which the effective electron-ion interaction had no Coulomb asymptotics in the ion core region, but was represented by a momentum dependent constant values, that provided the nonlocal form of pseudopotential.

Namely the model approach in the theory of pseudopotentials was in the focus of Z.Gurskii's Ph.D. studies. Model pseudopotentials were needed in order to exclude core electron states from the treatment in electron-ion Hamiltonian and represent the wave functions of lowest valence electrons as nodeless orbitals. Z.Gurskii and G.Krasko proposed a new model pseudopotential, which in contrast to the Heine-Abarenkov effective potential was an analytical continuous function inside and outside the ion core region. Simplicity of analytical form and fast convergence of perturbation expansions provided the success and wide applicability of this effective electron-ion potential, which very soon has been named in the literature as Krasko-Gurskii pseudopotential.

After the return to Lviv in 1970 Z.Gurskii started his scientific career at the Lviv Department of statistical theory of condensed states from the Kyiv Institute for Theoretical Physics, created just in 1969 in Lviv by N.Bogolyubov and headed by I.Yukhnovskii. In 1971 Zinoviy Gurskii received his Ph.D. degree from I.Franko Lviv State University defending the thesis entitled "A method of model pseudopotentials and some atomic properties of simple metals".

The pseudopotential theory remained in the focus of Z.Gurskii's research after Ph.D. defence, but he turned to the problems of first-principles pseudopotentials of Phillips-Kleinman type, which due to the overcompleteness of the set of orthogonalized plane waves displayed numerical instabilities in calculations with large number of basis functions. Using the original idea by M.Girardeau (1971) Zinoviy Gurskii together with his brother Bohdan formulated a mathematical formalism of completely orthogonalized plane waves (COPW). The pseudopotentials obtained in the COPW formalism did not depend on the sought electron energy as it was in the case of Phillips-Kleinman pseudopotentials. At that time the COPW approach was the only mathematically exact form of *ab initio* effective electron-ion interactions obtained from atomic Hamiltonian via unitary transformation in order to get rid of the core electronic states. Unfortunately these results by Gurskii brothers were not published in regular international journals, that would bring them wide recognition. Much later, only in 1992 L.Kleinman and D.M.Bylander proposed similar unitary transformation with the purpose of obtaining the so-called "exact Phillips-Kleinman-like pseudopotential".

Starting from the late 70-s Z.Gurskii got interested in physics of disordered systems and electronic processes in transition metals. Active research on the applicability of pseudopotential theory to liquid metals received high recognition. In 1983 Zinoviy Gurskii together with a group of physicists from the I.Franko Lviv State University received the State Award of Ukraine for a series of works entitled "Experimental and theoretical studies on physics of liquid metals".

In parallel to the development of pseudopotential method, Z.Gurskii worked on the theory of phase transitions and the problems of phase diagram calculations for binary alloys. A statistical theory free of phenomenological parametrs, which described the substitutional alloys in a wide range of temperatures, pressure and concentrations, was created using the method of collective variables. This theory permitted to estimate a critical region and to predict the behaviour of thermodynamic functions in binary alloys close to the temperature of phase transition order-disorder. In 1985 Z.Gurskii received the degree of Doctor of Sciences from the M.Lomonosov Moscow State University for the thesis entitled "A method of pseudopotentials in theory of metals and alloys". Later on all these results in pseudopotential theory and statistical theory of binary alloys were put together in the book "Quantum-statistical theory of disordered systems" (Kyiv,Naukova Dumka,1991) written together with Professor I.Yukhnovskii.

Important results were obtained by Z.Gurskii and his group in the studies of lattice dynamics in disordered alloys. The standard approach in the framework of coherent potential approximation did not take into account the fluctuations in local structure around the atoms in disordered alloys. A simple and effective approximation of a mean correlated crystal was proposed and successfully used in accounting for the effects of short-range order in collective dynamics of disordered binary alloys. There were explained the features of a high-frequency region in the phonon density of states for disordered alloys at low temperatures, when the effects of short-range order became essential close to the temperature of phase transition order-disorder. Z.Gurskii developed a microscopic approach which accounted for the effect of local atomic static displacements on the thermodynamics of binary alloys. A new equation for amplitudes of atomic static displacements was obtained, which permitted to perform calculations of the amplitudes from the first principles.

Since 1999 Zinoviy Gurskii has been a visiting Professor at the Opole University in Poland. During this period his interests concerned many-particle interactions in metals, construction of spin-dependent interatomic potentials in transition metals and studies of thermal atomic vibrations in the thermodynamics of binary alloys.

Up to his last days Professor Gurskii was head of the Department for Theory of Metals and Alloys at the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine. Over three decades of his scientific career Z.Gurskii published numerous papers in Ukrainian and international journals. He was the member of the editorial boards of the journals "Condensed Matter Physics" (Lviv) and "Progress in Physics of Metals" (Kyiv). Professor Z.Gurskii was a supervisor of eight successful Ph.D. works and a scientific adviser of two research works for Doctor of Sciences degree. Being a very intelligent and sincere person Zinoviy Gurskii was always open for discussions and advice. He created an atmosphere of warm human relations in his Department that provided successful work of the group. Unfortunately a heavy illness stopped the life of this extremely intelligent and very warm person. Many of the unfinished ideas by Zinoviy Gurskii are being further developed by his colleagues and followers.

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Selected publications by Z.Gurskii

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