

crystallographers

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Valentin Ivanovich Simonov (1930-2012)

Professor Valentin Ivanovich Simonov, a prominent scientist and organizer and a renowned expert in the field of structural crystallography, passed away on 23 February 2012. He was born on 8 March 1930 in the small town of Nizhne-Chirskaya of Volgograd region. In 1955, he graduated from the Department of Physics and Mathematics of Gor'kii (nowadays Niznii Novgorod) State University, where he studied at the chair headed by the academician N. V. Belov. From 1955 to 1958 he was Belov's postgraduate student at the Institute of Crystallography of the USSR Academy of Sciences, Moscow, and then started to work at Belov's laboratory. In the Institute of Crystallography he rose from research assistant to become head of the X-ray analysis laboratory and Deputy Director. From 1996 to 1998 he served as Director of the institute. Until the last day of his life Valentin Ivanovich continued to work actively in the position of Scientific Adviser of the laboratory of X-ray analysis techniques and synchrotron radiation.

Simonov was a recognized expert in structural crystallography. His contribution to the development of methods in this field of research, to the automation of crystallographic studies and to solving the problems of the structural conditionality of physical properties of crystals has been recognized in Russia and abroad. Simonov developed modern superposition methods for studying the atomic structure of crystals based on diffraction data. He also proposed and brought to fruition the concept of combining direct interpretation of the function of interatomic vectors with an analysis of Fourier expansion coefficients for electron density, which helped solve the central problem of structural analysis: refining structural amplitude phases. Corresponding software has been developed for Simonov's methods, and this is currently being used in structural research. The methods developed by Simonov were always aimed at solving specific structural problems for crystals interesting for solid-state physics, chemistry, mineralogy and materials science.



Figure 1 Valentin Ivanovich Simonov (1930–2012).

Twenty-three young experts have successfully defended their PhD theses under Simonov's supervision; some of them became Doctors of Sciences later. Now his students work not only in Moscow but also in Vladivostok, Ulan-Ude, Krasnoyarsk, Nizhnii Novgorod, Saransk, and some of them in Poland, China and South Korea. They actively use crystallographic methods in solving various problems of solid-state physics, chemistry, mineralogy and materials science.

For a long time Simonov was a member of the Scientific Council on Condensed Matter of the Russian Academy of Sciences and the Vice-Chairman of the National Committee of Russian Crystallographers. Simonov was a member of the Executive Committee of the International Union of Crystallography (1978–1984) and Vice-President of this organization (1984–1987). He was also co-opted as an ordinary member of the Executive Committee (1989–1990) following the death of S. A. Semiletov.

Simonov was actively involved in international scientific cooperation when computers became available for crystallographers. At that time the International Union of Crystallography organized a Commission on Crystallographic Computing, and Simonov became one of its members. Later he was elected a member of the editorial board of one of the oldest crystallographic journals: *Zeitschrift für Kristallographie*. For many years V. I. Simonov was a member of the editorial boards of the journal *Kristallografiya* (*Crystallography Reports*). For 12 years he worked as a Co-editor of *Acta Crystallographica*. He was a member of the Commission on Journals from 1979 to 1996.

Simonov's successful activity in science has been highly valued. He was granted the honorary title 'Honored Scientist of the Russian Federation' and awarded a Badge of Honor and a medal 'For Merits to Motherland' for his scientific achievements. In 1992, Simonov was awarded the prestigious Fedorov prize of the Russian Academy of Sciences. Until the very end Simonov was actively working on methods for studying the atomic structure of nanoinclusions in crystals. Information about the structure of such clusters, nanocrystals and nanoparticles on the whole is present in continuous X-ray diffuse scattering. Simonov and his colleagues (mathematicians) were engaged in a generalization of the Patterson methods for studying such objects and all his plans for the future were related to the development of this direction.

Scientific work has always been the meaning of life for Valentine Ivanovich. He perceived worries and concerns of the institute and the laboratory as his own and generously passed on his knowledge and experience to his students and colleagues. Everyone who worked with him deeply grieves and feels it as an irreparable loss.

Group of colleagues