Pushing Boundaries: Symposium Honors the Contributions of Vasek Vitek

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Editor's Note: For a more detailed look at Vitek's work, read the full article on MaterialsTechnology@TMS at <http://materialstechnology.tms.org/EMT/article.aspx?articleID=2749>.

Vasek Vitek was exploring largely uncharted territory as he toiled on atomistic simulation of dislocations and stacking faults in the wee hours of the morning at Oxford University in the late 1960s.

At that time, one computer served the entire university, and as a postdoctoral fellow, the only way Vitek could ensure access to it for his studies was to “spend a lot of nights there,” sometimes not going to bed until 6 a.m. to snatch a few hours sleep.

What emerged from Vitek's marathon late-night sessions would help lay the groundwork for today's field of computational materials science. In the words of his first Ph.D. student, Adrian Sutton, “When Vasek began his simulations of screw dislocations in the '60s, there were very few people anywhere in the world engaged in such work. Metallurgy, as materials science was known then, was largely an empirical subject dominated by experimentalists, with a few theorists working with pencils and paper. Today, we regard computational materials science as one of the central pillars of the subject, and there are thousands of people engaged in the pursuit. Vasek has contributed directly to that transformation through his own seminal research. He is a father figure in computational materials science.”

To recognize Vitek's influential contributions to materials science and engineering, Sutton, currently professor

of Nanotechnology at Imperial College London, and a number of other colleagues are organizing the “The Vasek Vitek Honorary Symposium on Crystal Defects, Computational Materials Science, and Applications,” scheduled for the TMS 2010 Annual Meeting in Seattle, Washington, February 14–18.

“Our goal is to bring together scientists from across the areas of materials science that have been impacted by Professor Vitek's work,” said David J. Srolovitz, symposium co-organizer and director of the Institute for Advanced Computing in Singapore. “While the areas are diverse, the approach, the methodology, and the type of thinking that he has taught all of us in this field are common across the topics we cover in this symposium. It is our hope that these commonalities are brought into sharp focus by examining Professor Vitek's contributions as a whole.”

It was as a postdoc at Oxford that Vitek wrote his most cited paper, which introduced the concept of the gamma-surface (V. Vitek, *Phil. Mag.* 18, (1968) p. 773). “This is a theoretical construct so fundamental to the understanding of the mechanical properties of materials that it is taught routinely during undergraduate degrees,” said Marc Cawwell, a recent Ph.D. student of Vitek's who is currently working at Los Alamos National Laboratory.

Vitek's pioneering studies “paved the way for many subsequent atomistic simulations of the structure and motion of dislocations in b.c.c. metals, using more realistic potentials for transition metals and ab-initio computation,” said Peter Hirsch, Emeritus Professor of Metallurgy at Oxford, who was the Isaac Wolfson Professor of Metallurgy and head of the department at the university when Vitek joined it in 1967. Petros Sofronis, professor and Asso-

ciate Head for Mechanics Programs, University of Illinois at Urbana at Champaign, likewise described Vitek as “a path-breaker in any area of mechanical behavior of materials he has worked on,” with “seminal and novel” contributions in the area of solid mechanics.

“Vitek's characteristic contribution has been to show how computer simulations on the atomistic scale can be used to further our understanding of structures of defects and of mechanical properties of metals and alloys, opening a new and powerful approach in this field,” said Hirsch. “He is, without doubt, a world leader in this area, and his work has had considerable impact.”

Over the years, numerous accolades have been showered upon Vitek, a professor at the University of Pennsylvania since 1978. However, he attributes the path that his career has taken to the mentors and colleagues who have helped shape him along the way. He credits Franta Kroupa, his Ph.D. advisor at the Czechoslovak Academy of Sciences, for introducing him to the study of the mechanical behavior of materials, and points to his postdoctoral advisor at Oxford, J.W. Christian, for “helping me develop really independent thinking—to not follow fashions in science.” He also notes that he “is deeply indebted” to Hirsch, “not only for profound scientific advice, but also for his help after the Soviet invasion of Czechoslovakia that impacted my whole life.” As to the future of materials science and engineering, Vitek said that predicting truly new directions in the field is “almost impossible.”

“If I were able to tell you, it would not be a breakthrough,” he said.

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