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Materials Science Needs and Is Getting Quantitative Methods FREE

Gerd Ceder; Jerzy Bernholc

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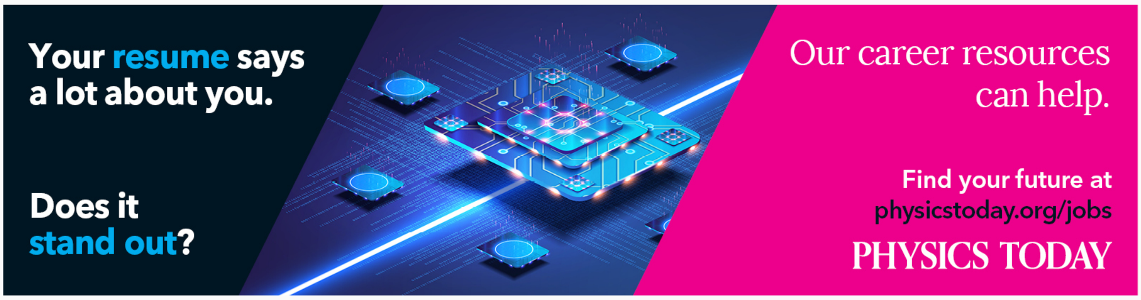

LETTERS

(continued from page 15)

Lawrence Cranberg compares Oppenheimer with Fermi. As postdoc of the former's and student of the latter's, I feel that some thing should be said. Certainly Fermi was a marvelous model for a physicist, and I don't know who could stand the comparison. Cranberg blames Oppie for not being, as Fermi was, successful in experiment as well as theory. But who else was? Einstein? Feynman? Schwinger? Von Neumann? In this, Fermi was probably unique in our century. Cranberg credits development of the A-bomb to President Roosevelt, and its use to President Truman, and he takes Oppie to task for not having made any technical contributions.

I am not happy that the bomb was developed, and much less so that it was used, and I do not admire Oppie for having been the director of the project. But I have only heard good things about his wartime direction of Los Alamos, never any criticism. In fact, from all that I have read, Oppie was an excellent director. And before the war, he had been *the* outstanding leader and teacher of theoretical physics in the US. He brought into existence the first American school of theoretical physics. As a student just after the war, I still studied quantum mechanics from prewar mimeographed notes of an Oppenheimer course (the teacher of my course was Edward Teller). As a young postdoc at the Institute for Advanced Study in Princeton in 1948–49, where Oppie was the director, I—like others interested in field theory and in particle physics—eagerly attended the weekly seminars he organized.

In short, denying Oppenheimer's leading role in physics, especially in US physics, is hardly correct.

JACK STEINBERGER
(jack.steinberger@cern.ch)
CERN
Geneva, Switzerland

CRANBERG REPLIES: I welcome the responses of Timothy Karpin, James Osborn, and Jack Steinberger. To add useful evidence and analysis to the A-bomb story, though, I too think it best to cite sources. My reading of Richard Rhodes, for example, is that he attributes the "Los Alamos Primer" to lectures given by Robert Serber and compiled by associate lab director Edward Condon.[1] J. Robert Oppenheimer's role was evidently to convene the lectures. Further, Rhodes states that implosion, the key development beyond the "Los Alamos Primer" phase, is attributable to Seth Neddermeyer, and Rhodes quotes John Manley, who was there, as saying that Neddermeyer faced "stiff opposition" from Oppenheimer and others.[2]

I stand by my original letter, but that letter will have served a higher purpose than evaluating Oppenheimer's role in the A-bomb project if it focuses attention on the underlying and recurring general questions about the requirements for leadership of large-scale scientific-engineering endeavors. And I hope that both the letter and this exchange will continue to stimulate constructive discussion of those requirements—surely a topic worthy of further discussion in the pages of both PHYSICS TODAY and *APS News*.

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LAWRENCE CRANBERG
Austin, Texas

Does H_0 Play Role in Universe Like h Does in Atomic Domain?

Of the many redshift studies that have been done over the years, one of the most interesting has to be that of William Tifft of the Steward Observatory in Arizona. He has been studying and reporting on redshift data for over two decades now, and has repeatedly found a bunching of the data around certain values.[1] When interpreted in terms of recessional velocities in the usual way, these values are integral multiples of a certain basic value—namely, 72 km/s. Although somewhat controversial initially, these basic results were later confirmed by Bruce Guthrie and William Napier of the Royal Observatory in the UK.[2]

Furthermore, these results have also proved to be very close to the latest value reported for the Hubble constant, as announced by the Hubble Space Telescope H_0 Key Project team: 71 km/s per megaparsec (see PHYSICS TODAY, August 1999, page 19). Here it is useful to note that, in her 1992 survey,[3] team coleader Wendy Freedman gave the most probable value of H_0 as 73 km/(s Mpc).

The closeness of all of the above results suggests that the recessional velocities measured by Tifft could be written as integral multiples of H_0, so that $v = n \cdot H_0 d_0$, where n is an integer and d_0 is a basic unit of distance (1 Mpc). This equation is basically a quantized form of Hubble's law, and it implies that galaxies are located only at certain distances $d = nd_0$ away from us, at least in the near universe. Just how far out this equation would apply is not clear, but it does hold for our nearest galactic neighbor, M31 (the Andromeda galaxy), which is known to be approximately 1 Mpc away (corresponding to $n = 1$ in the above formula).

A quantized Hubble's law might be masked by other effects farther out, but it does suggest that the Hubble constant may play a role in the large-scale universe similar to that played by Planck's constant in the atomic domain—that is, in giving rise to structure in the universe.

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MAURICE T. RAIFORD
(mtr@physics.ucf.edu)
University of Central Florida
Orlando, Florida

Materials Science Needs and Is Getting Quantitative Methods

The following comment is prompted by my having read Jerzy Bernholc's article, "Computational Materials Science: The Era of Applied Quantum Mechanics," in your September 1999 issue (page 30). Although we must be impressed by the ingenuity that is often displayed in large-scale *ab initio* simulations, the road from breaking a solid or molecule in a simulation to the engineering concept of "strength" is a long one, and unlikely to be traversed by using simulations only. Similarly, other relevant engineering properties, such as corrosion and fracture resistance, phase (meta)stability, microstructure formation, and macroscopic transport, are often a complex (and unknown) combination of microscopic phenomena.

What is the problem? Due to the

lack of microscopic information, the discipline of materials science and engineering has historically developed as an empirical and nonquantitative one. Now that advances in computational quantum mechanics have made detailed microscopic information available, we find ourselves searching for quantitative materials theories with which to integrate them. The true challenge, therefore, is to develop theories that will lead to the systematic coarse graining of microscopic phenomena into macroscopic behavior. The problem, then, is one of detailed knowledge of the phenomena at the intermediate scale, rather than one of computational quantum mechanics.

GERD CEDER
(gceder@mit.edu)
Massachusetts Institute of Technology
Cambridge, Massachusetts

BERNHOLC REPLIES: Although many problems can be addressed solely by atomistic simulations, there are many that cannot be, due either to the length or time scales involved. As Gert Ceder points out, empirical and nonquantitative models provided and continue to provide important guidance in such cases. However, one of the main emerging theoretical thrusts consists of multiscale methods, in which microscopic information from atomistic simulations is combined with continuum mechanics or Monte Carlo methods to obtain the required coarse graining. (The first—and too long—draft version of my article did contain a section on such methods.)

Although multiscale methods are still emerging, good progress is being made.[1] Ideally, multiscale calculations would proceed in a manner analogous to the multigrid method, in which the information from the coarsened solutions is used to recursively accelerate the progress on the finer scales. Conversely, the fine-scale solutions improve the accuracy of the coarsening. However, a number of methodological aspects still need to be developed.

Turning to the specific example of "strength," let's focus briefly on the nanotube example discussed in my article. *Ab initio* and classical simulations[2] predicted that nanotubes would be thermodynamically stable at strains up to 5–6%, and kinetically metastable at significantly greater strains. Although it has not yet been possible to simulate the entire fracture process at realistic timescales, the "minimum strength" prediction is still quite useful. Recent measurements made by Richard Smalley's[3] and Charles Lieber's groups show that carbon nanotubes can sustain at least a 5% strain—making them the "strongest" material known!

I must also point out that the progress made in computer science affected my article in another, much less desirable way. My overconfident computer spelling checker changed Alex Zettl's name to Alex Seattle, and I, for one, feel profoundly sorry and apologize for failing to read the corrections one more time.

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JERZY BERNHOLC
(bernholc@ncsu.edu)
North Carolina State University
Raleigh, North Carolina

More on History of *P, CP, T* Violation in Strong Interactions

In her story entitled "Going for the Gold: First Collisions at RHIC Are Set for December" (PHYSICS TODAY, October 1999, page 20), Gloria Lubkin mentions a 1998 proposal by Dimitri Kharzeev, Robert Pisarski, and Michel Tytgat that a *P*- and *CP*-violating metastable state could be produced in heavy-ion collisions. I would like to inform your readers that the original idea for *P, CP*, and *T* violations in heavy-ion collisions due to the local excitation of the vacuum into an excited state that has the possibility of being *CP* violating was given in a 1985 paper by Peter D. Morley and myself.[1]

Reference

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IVAN SCHMIDT
(ischmidt@fis.utfsm.cl)
Technical University "Federico Santa Maria"
Valparaiso, Chile

Kharzeev, Pisarski, and Tytgat reply: We were previously unaware of the work of Peter Morley and Ivan Schmidt, and we are grateful for having it brought to our attention.

To the best of our knowledge, the possibility of spontaneous *P, CP*, and *T* violation in strong interactions is attributable to T. D. Lee, as reported in his 1973 paper, "A Theory of Spontaneous *T* Violation."[1] In a modern context, Lee considered an η' condensate, which is equivalent to a region with a nonzero θ angle. For example, his η' condensate induces a nonzero electric dipole moment of the neutron (equation 49) and *P*- and *CP*-odd contributions to hadron–hadron scattering amplitudes (equation 48).

In two 1974 papers,[2] Lee, and Lee and Gian Carlo Wick, discussed how metastable vacuum states, such as those with $\langle \eta' \rangle \neq 0$, arise in effective hadronic theories, and can form abnormal states of hadronic matter.

In their 1985 paper,[3] Morley and Schmidt discussed how *P, CP*, and *T* violations can arise in heavy-ion collisions from regions in which $\theta \neq 0$, but they did not offer a mechanism by which such regions could be generated. Although they did propose a signature—a spin correlation between outgoing protons—it remains a challenging task to measure this correlation experimentally.

In contrast, in our 1998 paper,[4] we propose a detailed dynamical mechanism of spontaneous *P* and *CP* violation. In both that paper and a subsequent work,[5] we also suggest how this effect would manifest itself in *P*- and *CP*-odd correlations of charged pions in heavy-ion collisions, which are measurable on an event-by-event basis.

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DMITRI KHARZEEV
(kharzeev@bnl.gov)
ROBERT PISARSKI
(pisarski@bnl.gov)
Brookhaven National Laboratory
Upton, New York
MICHEL TYTGAT
(michel.tytgat@cern.ch)
Free University of Brussels
Brussels, Belgium ■