

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.

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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 simulations² 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’s³ 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.

References

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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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Kharzeev, Pisarski, and Tytgat reply: We were previously unaware of the work of Peter Morley and Ivan Schmidt, and we are grate-

ful 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.

References

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