Ultrafast phase transitions in advanced materials, including light-induced superconductivity

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We begin by reviewing some experimental studies of advanced materials responding to femtosecond-scale laser pulses, with an emphasis on ultrafast phase transitions. One motivation for the experiments, and for the theoretical approaches described below, is that the dynamical response can help to discriminate among possible mechanisms for an observed phase transition. A paradigm is the metal-insulator transition in VO_2; if it is primarily an electronic Mott-Hubbard transition, rather than a structural Peierls transition, the time scale may be roughly two orders of magnitude shorter – femtoseconds rather than hundreds of femtoseconds. The dynamics of phase transitions in the cuprates and iron-based high-Tc materials may provide information on the mechanism of superconductivity, which is still an unsolved problem despite the claims of success for various different theoretical models. In particular, we will discuss the apparent observations of light-induced superconductivity in cuprates and doped fullerenes. In one set of experiments [1], the interpretation is that stripe ordering is a competing phase, and "melting" of the stripes permits the emergence of 3-dimensional superconductivity.

We introduce a new method for treating ultrafast phase transitions, such as those involving superconductivity, magnetism, charge density waves, and spin density waves. This method is made possible by the fact that the density-functional-based technique emphasized here (and also standard density-functional approaches and other first-principles techniques, as long as they include nuclear motion) can yield a true electronic temperature [2]. Illustrative results will be presented for a simple model, with the electronic temperature immediately after the laser pulse calculated as a function of the fluence. In addition, we describe two other complementary approaches. In the first of these, phenomenological Landau-Ginzburg-like order parameters are coupled to one another and to the vector potential of the laser pulse. In the third and most ambitious approach, a self-energy is included in the time domain.

[1] D. Fausti, R. I. Tobey, N. Dean, S. Kaiser, A. Dienst, M. C. Hoffmann, S. Pyon, T. Takayama, H. Takagi, and A. Cavalleri, Light-Induced Superconductivity in a Stripe-Ordered Cuprate, Science 331, 189 (2011).

[2] Zhibin Lin and Roland E. Allen, Ultrafast equilibration of excited electrons in dynamical simulations, J. Phys. Condens. Matter 21, 485503 (2009).