PπIntertwined CDW and Defect Ordering Phase Transtions in a 2-D Stystem

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Last year at the Beijing Asia-Pacific Surface and Interface Analysis Conference I presented a talk titled “”Defect Mediated Phase Transition in 2-D: From Charge Density Waves to Defect Density Waves.” It this presentation the experimental data for the CDW formation in the a phase of the Sn/Ge(111) systems was described as well as the defect-defect interaction via the CDW forming a defect density wave was presented [1-3]. This year I will describe our effort to model these two intertwined phase transitions [4]. We present a model for the symmetry lowering phase transition in 2D systems such as Sn/Ge(111), Pb/Ge(111) and similar. Charge Compensation model (CCM) allows calculating the site dependent order parameter $q_{i.}$ for every site on the lattice depending on the defect distribution and temperature. This model is based on the minimization of free energy by iterating self-consistent set of equations, where the order parameter (“charge”) on every lattice site is calculated as a response to the “charges” on the nearest neighbors. Defects are assumed to have fixed “charge” and are treated as a boundary condition. Correct STM images can be simulated this way for the whole range of temperatures for a given defect distribution. This model system clearly exhibits critical behavior. The low temperature STM images have distinct features: sharp domain boundaries of the low symmetry phase. They can be very well reproduced in CC model but only if the temperature dependent parameter (“charge compensation factor”) has a value above critical. Below the critical value the calculated STM images appear as interference pattern of defect-induced exponentially decaying waves with the symmetry of the low temperature phase. The characteristic length of the exponential decay monotonically grows and diverges as the “charge compensation factor” approaches the critical value from below. This behavior reproduces experimentally observed pretransitional effects and evolution of the phase transition in Sn/Ge(111) [Melechko, 1999 #88]

The interaction of defects with defect-induced waves above the phase transition temperature leads to the defect-ordering phase transition, that accompanies the symmetry lowering phase transition. Such ordering is responsible for the domain size and shape at low temperatures. We modeled the alignment of defect assuming that they experience force exerted if there is a difference of the “charge” on the defect site and its nearest neighbor. The atoms exchange sites if this difference exceeds a threshold value. The characteristic length of the exponential decay of defect-induced waves was a main parameter in this simulation. The measure of order (“correlation probability”) has a sudden jump when the decay length exceeds a certain critical value. This corresponds to a transition from completely random defect distribution to defects aligned on one or two out of three sublattices. This behavior precisely reproduces the experimentally measured temperature dependent “correlation probability”.

1. Two-Dimensional Phase Transition Mediated by Extrinsic Defects, (A. V. Melechko, J. Braun, H. H. Weitering, and E. W. Plummer), Phys. Rev. Letters, **83**, 999 (1999).
2. Defect-Mediated Condensation of a Charge Density Wave, (H. H. Weitering, A. Melesko, J. M. Carpinelli, and E. W. Plummer), Science, **285**, 2107-2110 (1999).
3. The Role of Defects in Two-Dimensional Phase Transitions: an STM Study of the Sn/Ge(111) System, (A. V. Melechko, J. Braun, H. H. Weitering, and E. W. Plummer), Phys. Rev. B **61**, 2235 (2000).
4. Intertwined CDW and Defect Ordering Phase Transtions in a 2-D System, (A. V. Melechko, M. Simkin, N. F. Samatova, J. Braun, and E. W. Plummer), submitted to Phys. Rev. B.

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