

Surface Phase Transition Induced by Electron Mediated Long Range Interaction

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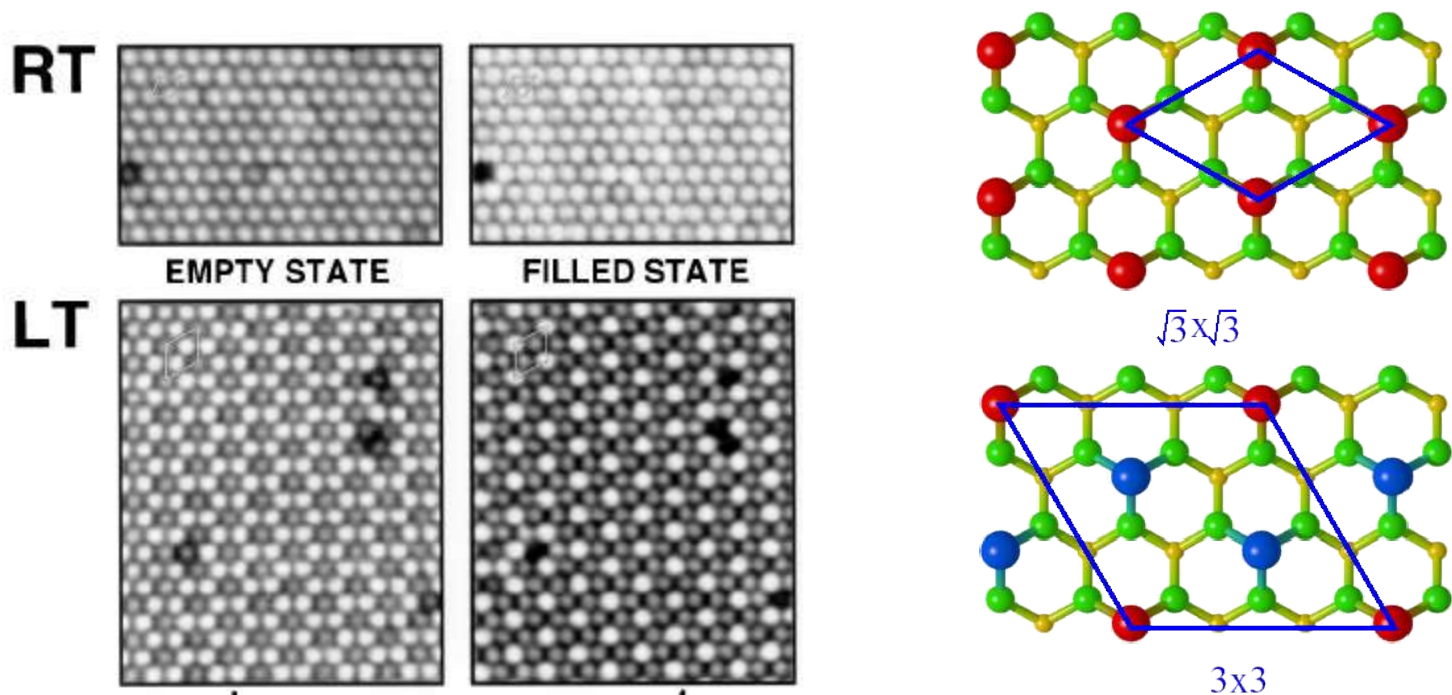
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University of Tennessee and ORNL

CDW in Sn and Pb on Ge(111)

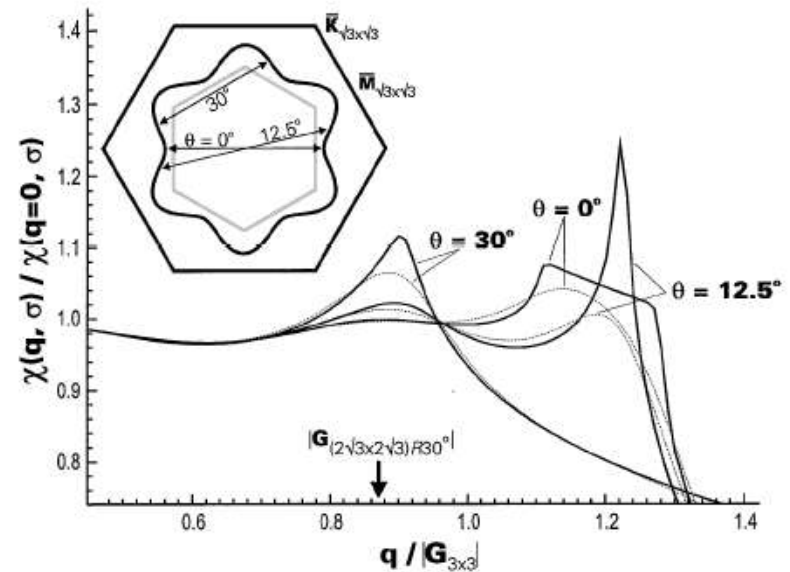


J.M. Carpinelli, H.H. Weiering, E.W. Plummer, and R. Stumpf,
Direct observation of a surface charge density wave.

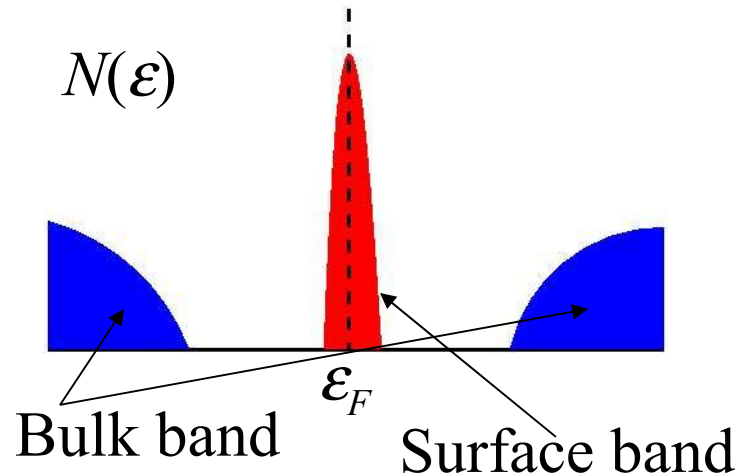
Nature **381**, 398 (1996).

Theoretical Speculations and Puzzles

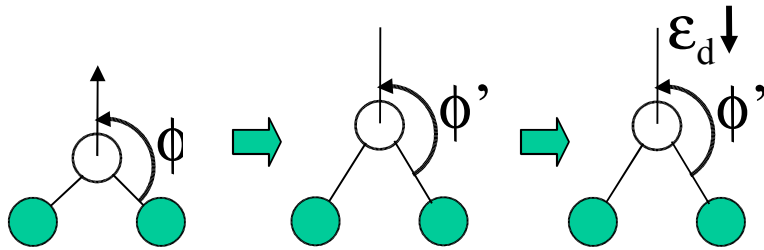
- Kohn Anomaly? -- no anomaly in response function
- Fermi surface nesting? -- no
- Surface Mott Insulator? – the surface is still metallic after the transition.
- Jahn-Teller effect?



What We Have

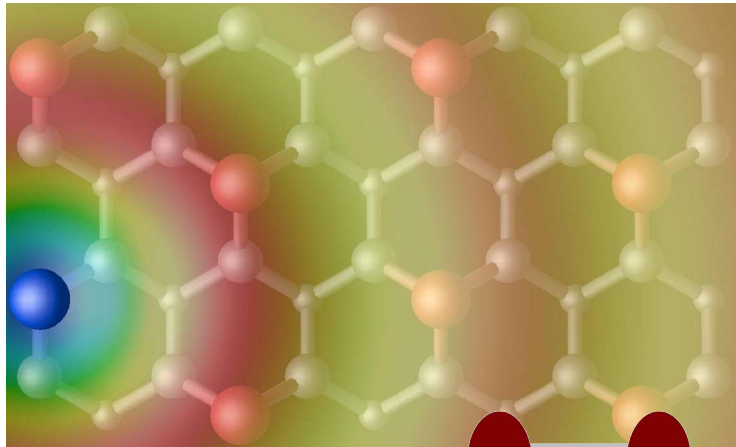


- Each Sn adatom has a dangling bond.
- The dangling bonds form a metallic surface.
- substantial surface density of states
- the strong electron-phonon coupling induced by the rehybridization between dangling bond and back bonds

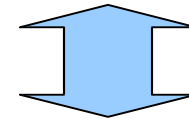


Origin of electron-phonon coupling.

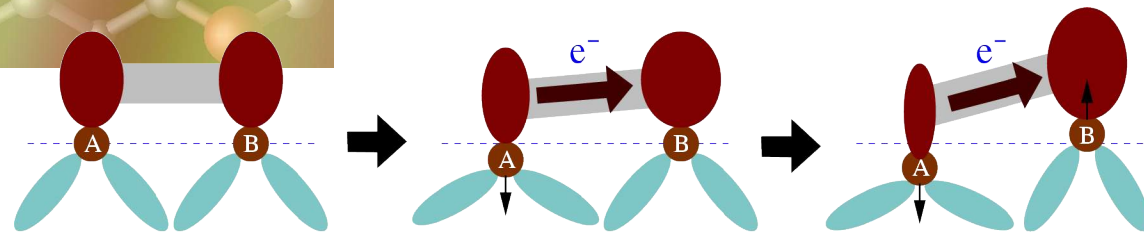
Our Theory: Electron Mediated Interaction



Adatom Displacement



Charge Corrugation



Competition: Local stress imposed by substrate keeps adatoms in their original positions.

Theories for the electron-mediated long range interaction:

Einstein and Schreiffer (1973); Lau and Kohn (1978)

T.T. Tsong (1973); Repp et al. (2000)

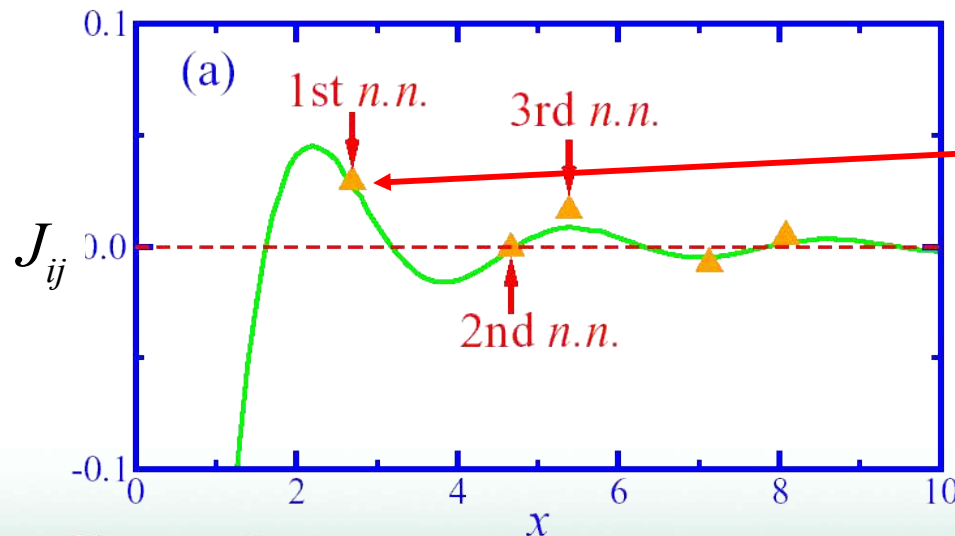
A Formal Theory

$$H = \sum_{is} (\varepsilon_0 - \beta z_i) c_{is}^\dagger c_{is} - t \sum_{\langle ij \rangle} (c_{is}^\dagger c_{js} + c.c.) + \frac{\alpha}{2} \sum_i z_i^2 + \dots$$

Dangling bond energy
change due to displacement

Local stress

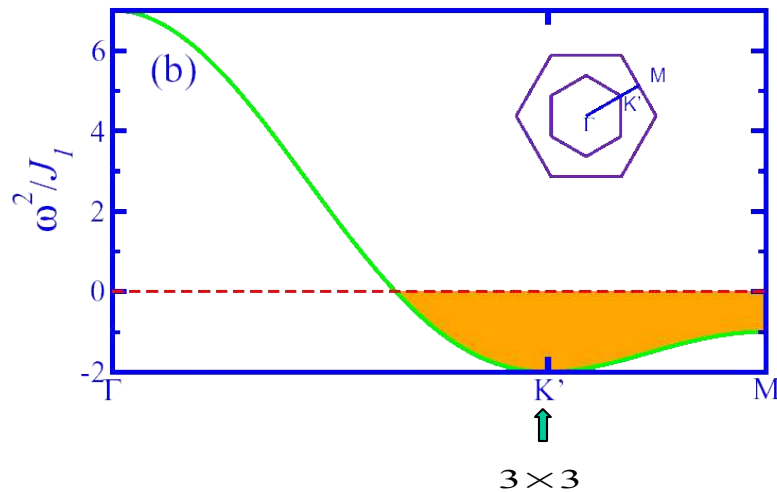
Effective Hamiltonian: $\Delta E = \frac{\alpha}{2} \sum_i z_i^2 - \beta \langle n \rangle \sum_i z_i - \frac{1}{4} \sum_{ij} J_{ij} (z_i - z_j)^2 + O(z^3)$



“Antiferromagnetic”-like coupling between neighboring adatoms!

$$J_{ij} \sim -\frac{\sin 2 k_F r}{r^2}$$

Consequence: Phonon Instability



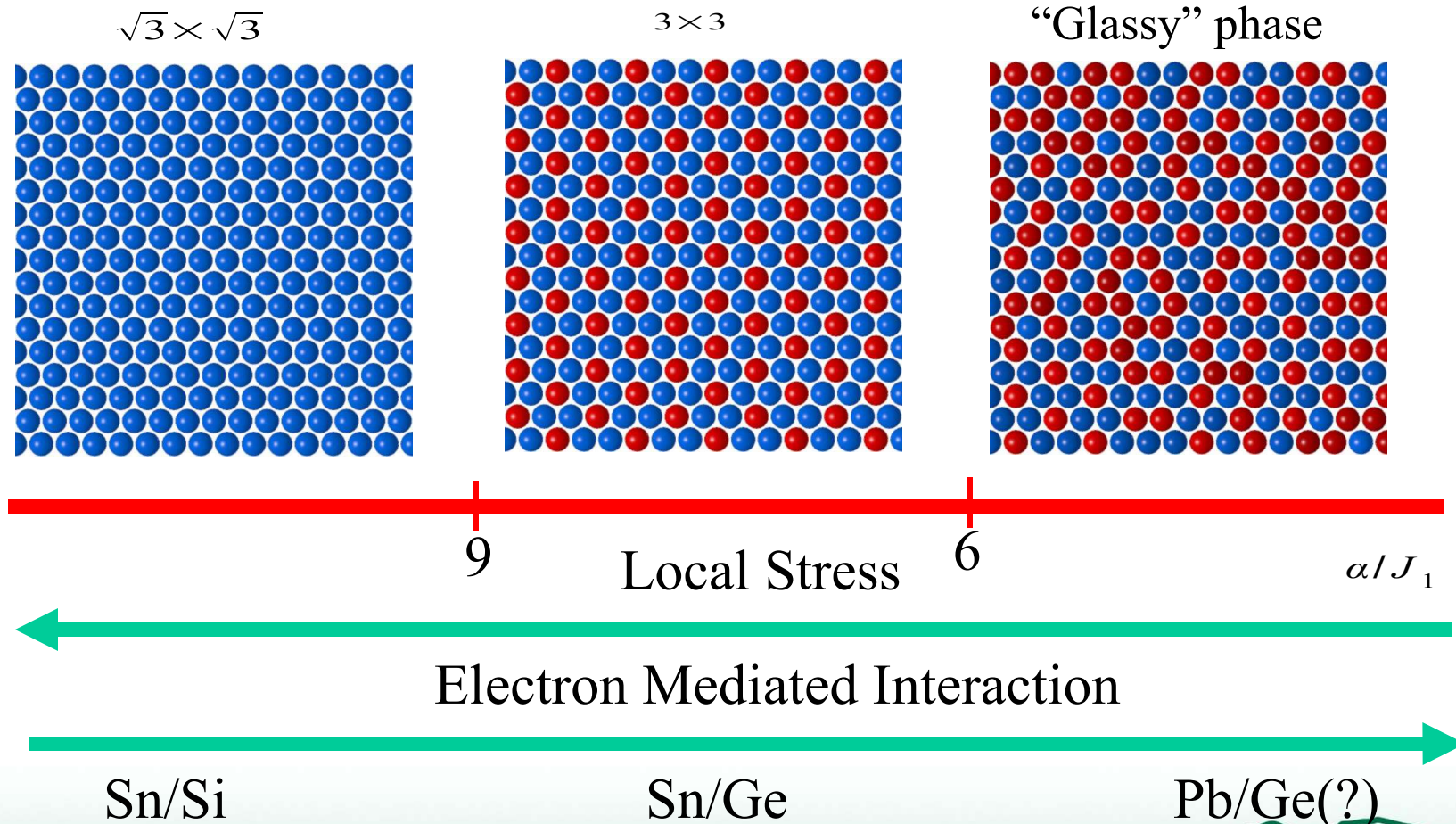
$$\Delta E = \frac{1}{2}(\alpha - 6J_1) \sum \tilde{z}_i^2 + \frac{J_1}{2} \sum_{\langle ij \rangle} \tilde{z}_i \tilde{z}_j + O(\tilde{z}^3)$$

$$\omega^2 = \alpha - 6J_1 + J_1 \sum_l \cos(\mathbf{k} \cdot \mathbf{R}_l)$$

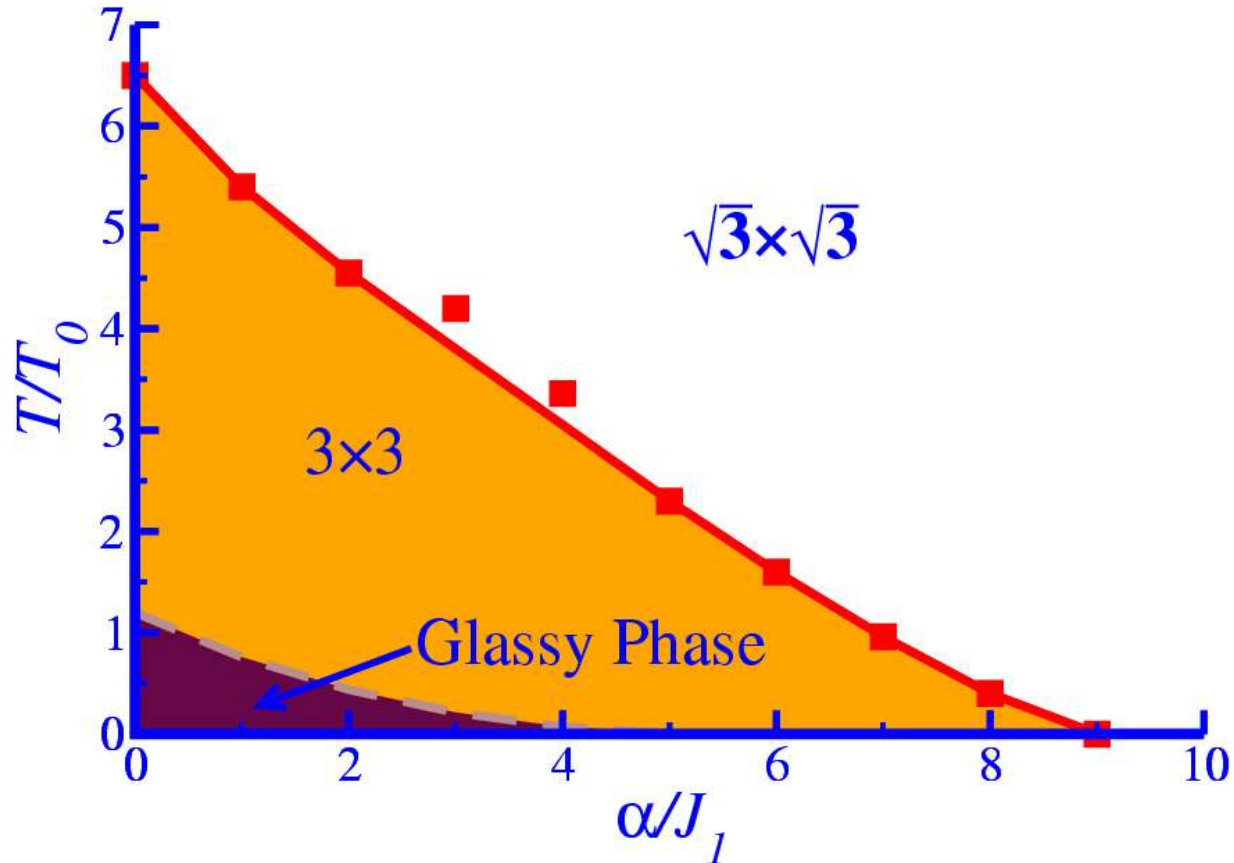
Phonon catastrophe

Transition occurs due to the phonon instability!

Ground States: Competition Between Local Stress and Electron Mediated Interaction

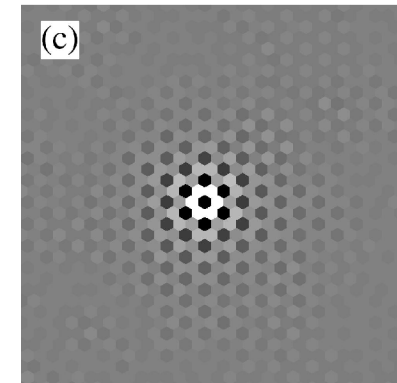
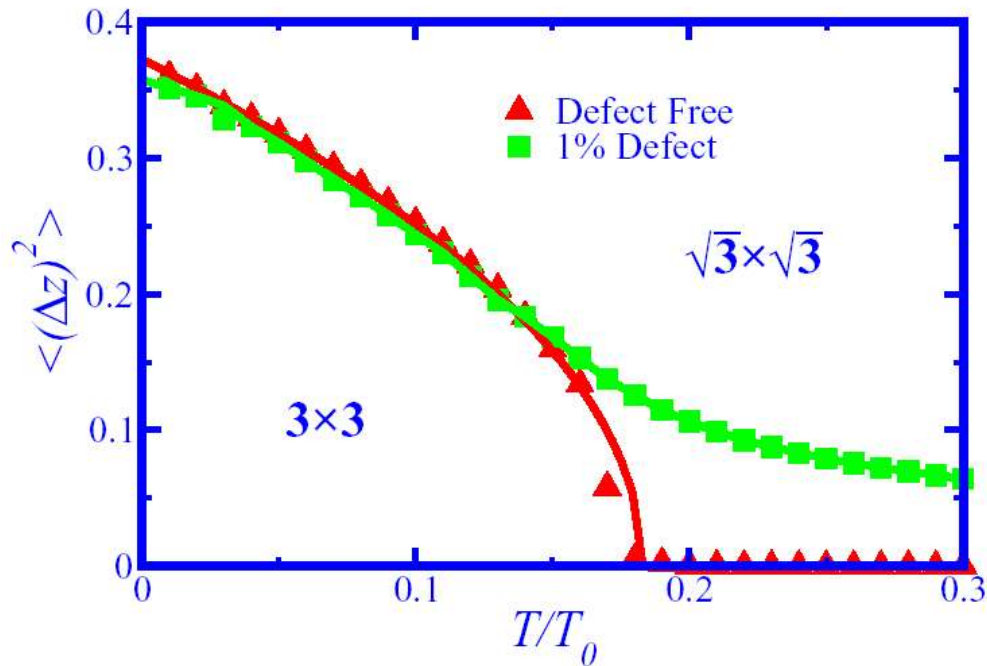


Phase Diagram

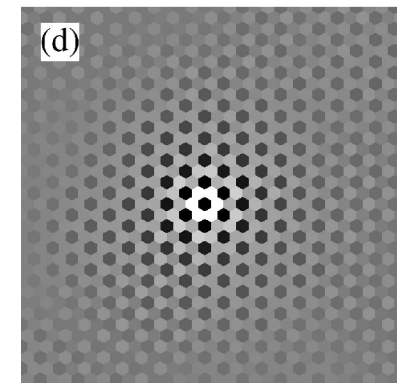


α : local stress J_1 : electron mediated force

Defect Blurred Transition



$T/T_c = 1.6$



$T/T_c = 1.1$

Summary

- The competition between local stress and electron mediated interaction results intriguing structural phase transitions.
- A high electron density of states and strong electron-phonon coupling are needed for the mechanism to work. In many surface systems, both are available.
- The mechanism could be applicable to other surface structural phase transitions, although the details may differ.