

# Condensed Matter Theory Center Seminar



Wednesday, June 24  
11:00 am – 12:00 pm  
2205 Toll Physics Building

## Noriko Akutsu

Osaka Electro-Communication University, Osaka, Japan

### “Phase Diagram of Step Faceting on a Crystal Surface: Numerical Calculations on a Restricted Solid-on-Solid Model with Point-Contact Type Step-Step Attraction”

The anisotropic surface tension of a vicinal (or slightly tilted) surface based on a solid-on-solid (SOS) model is calculated by a density matrix renormalization group (DMRG) method [1]. The SOS model we calculated is a restricted solid-on-solid (RSOS) model with point-contact-type step-step attraction (p-RSOS model) [2-5]. Here, “restricted” means that the height difference between the neighboring sites is restricted to 0, 1, and -1. The point-contact-type step-step attraction represents the energy gain which is obtained by forming a bonding state by the orbital-overlap at the meeting point of neighboring steps. The calculated surface tension shows discontinuity in slope dependence at low temperatures [3]. Due to the discontinuity, a step faceting phase [6] and a step droplet phase are formed [2, 3] in addition to the Gruber-Mullins-Pokrovsky-Talapov (GMPT) universal phase [4]. We show a phase diagram of these three phases [5].

- [1] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992). T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **64**, 4084 (1995). Y. Hieida, K. Okunishi and Y. Akutsu, Phys. Lett. A**233**, 464 (1997); New J. Phys. **1**, 7 (1999). U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).
- [2] Noriko Akutsu, Appl. Surf. Sci. **256**, 1205 (2009); J. Cryst. Growth **318**, 10 (2011).
- [3] Noriko Akutsu, J. Phys.: Condens. Matter **23**, 485004 (2011); Phys. Rev. E **86**, 061604 (2012); Phys. Rev. E online Kaleidoscope Image, December (2012); J. Cryst. Growth, **401**, 72 (2014).
- [4] E. E. Gruber and W. W. Mullins, J. Phys. Chem. Solids **28**, 6549 (1967). V. L. Pokrovsky and A. L. Talapov, Phys. Rev. Lett. **42**, 65 (1979). C. Jayaprakash, W. F. Saam, and S. Teitel, Phys. Rev. Lett. **50**, 2017 (1983). N. Akutsu and T. Yamamoto, *Handbook of Crystal Growth*, ed. T. Nishinaga, Vol. I. Elsevier (2015) pp. 265-313; T. L. Einstein, ibid., pp. 216-265.
- [5] Noriko Akutsu, in preparation.
- [6] W. W. Mullins, Philos. Mag. **6**, 1313 (1961). N. Cabrera, *Symposium on Properties of Surfaces*, p. 24 (Am. Soc. Testing and Materials, Philadelphia 1963); Surf. Sci. **2**, 320 (1964).

Host: Ted Einstein

Web: <http://www.physics.umd.edu/cmtc/seminars.html>

