

# MSE-Colloquium@NTU

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## Dynamic Grain Boundary Phase Transitions and their Microstructural Implications

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### Abstract

Grain boundaries (GBs) exhibit many different types of phase transformations associated with their distinct atomic structures. This is akin to phase transformation in bulk crystals, albeit in one few spatial dimensions. On the other hand, free surfaces exhibit roughening phase transitions that are associated with thermodynamic instabilities of their line defect - i.e., surface steps. GBs also contain line defects, known as disconnections, with both step and dislocation character (characterized by a step height  $h$  and a Burgers vector  $\mathbf{b}$ ).

I will present theoretical arguments, Monte Carlo, kinetic Monte Carlo, and molecular dynamics results that show the GBs undergo a roughening transition (like surfaces - associated with  $h$ ) and an elastic "screening" transition (unlike on surface - associated with  $\mathbf{b}$ ). At temperatures, below the screening transition disconnections have long range ( $1/r$ ) interactions, but above that, their interactions decay exponentially,  $\exp(-r/\xi)$  where  $\xi$  is a screening length. This is a Berezinskii-Kosterlitz-Thouless topological phase transition. I will explain this effect based upon a heuristic argument and supplement it with our recent renormalization group calculations of the transition temperature  $T_c$ . This phase transition has profound effect on GB migration - below the  $T_c$ , GBs are nearly immobile, while above this they are mobile. I will end by discussing the implications of this transition for grain growth.

### Biography

Dr David Srolovitz is the author of 500 papers on materials theory/simulations on defects, microstructure, deformation and film growth with an H-index of 94. He is a Member of the US National Academy of Engineering, Fellow of MRS, TMS, ASM, Institute of Physics and is the winner of the MRS Materials Theory Award. At various times, he was a staff member at A\*STAR (IHPC), Exxon Corporate Research and Los Alamos National Laboratory and was Professor at the University of Michigan, Princeton University, and the University of Pennsylvania. Dr Srolovitz is currently a Chair Professor at the City University of Hong Kong and a Senior Fellow of the Hong Kong Institute for Advanced Study.