Why is Iridium the best substrate for single crystal diamond growth?

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Outline

- Experimental situation
- Simulation results for Ir Re Si and Pt
  - Surface energies
  - Dissolution energies
  - Migration
  - A model for nucleation dynamics
- Conclusions

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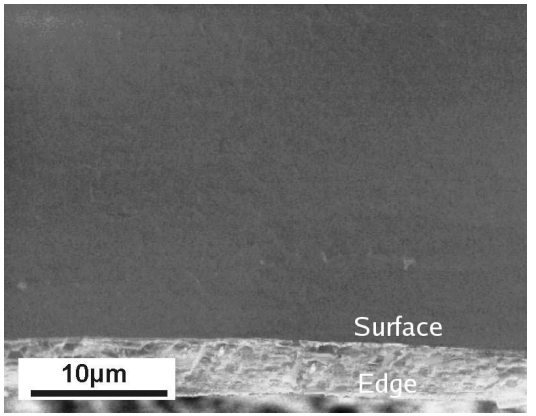
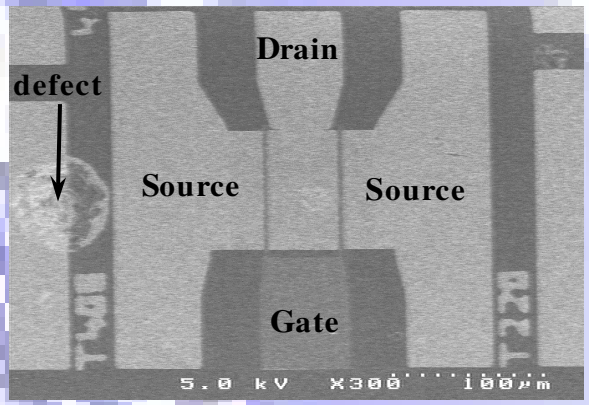
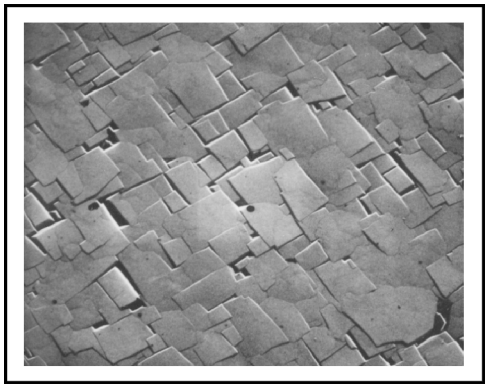
- Diamond is hard, good T conductor, large mobilities, resistance, semicond, and “dopable”
- Many substrates grow (100) diamond
- Crystallinity is expt 10 times better on Ir
- Re retains more C
- BEN is essential



Diamond on $Ir/SrTiO_3(001)$



FET M. Kubovic (Universität Ulm)



Diamond on silicon

- Experimental situation
- Simulation results for Ir Re Si and Pt
  - Surface energies
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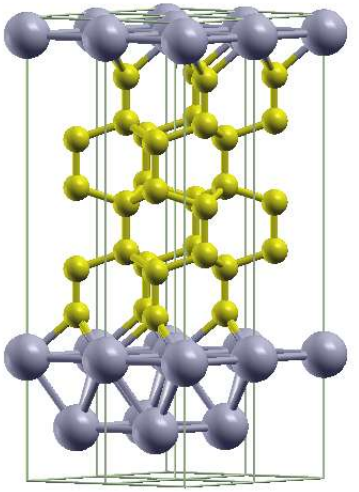
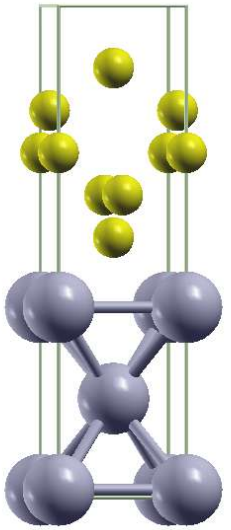
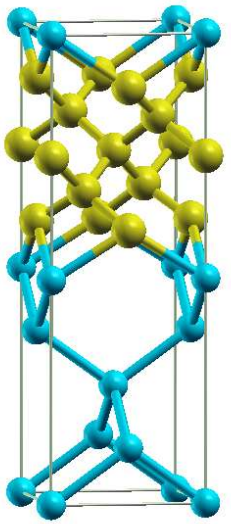
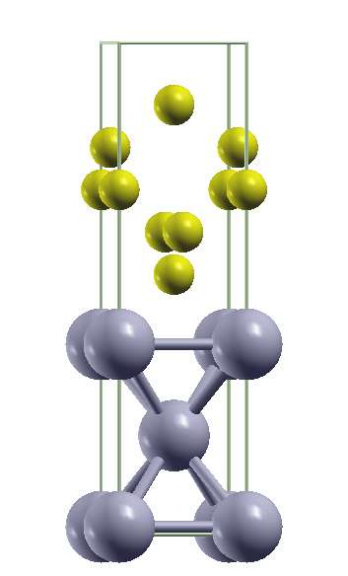
- Conclusions

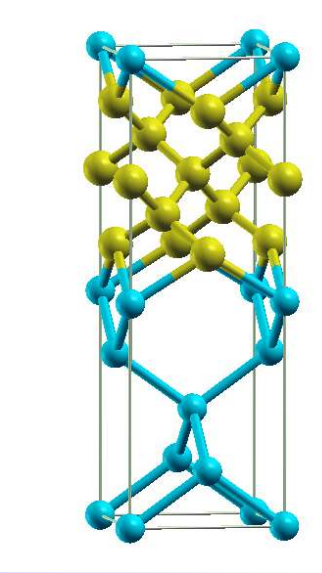
- Compare Ir, Re, Pt, Si
- Pt close to Ir, Si cheap, Re interesting
- Interface and dissolution energies
- Explain dynamics from equilibrium calculations
- Explain chemical difference between substrates

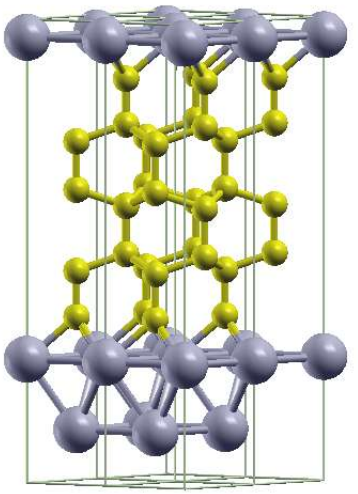




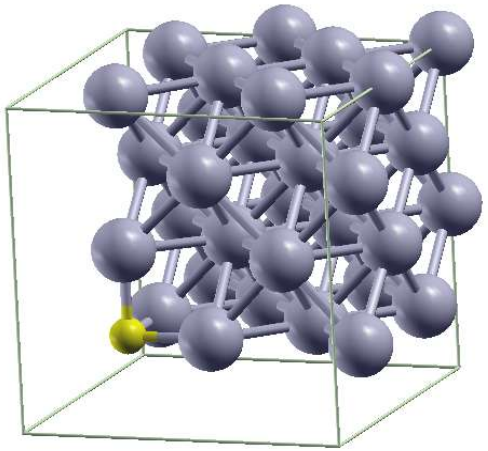


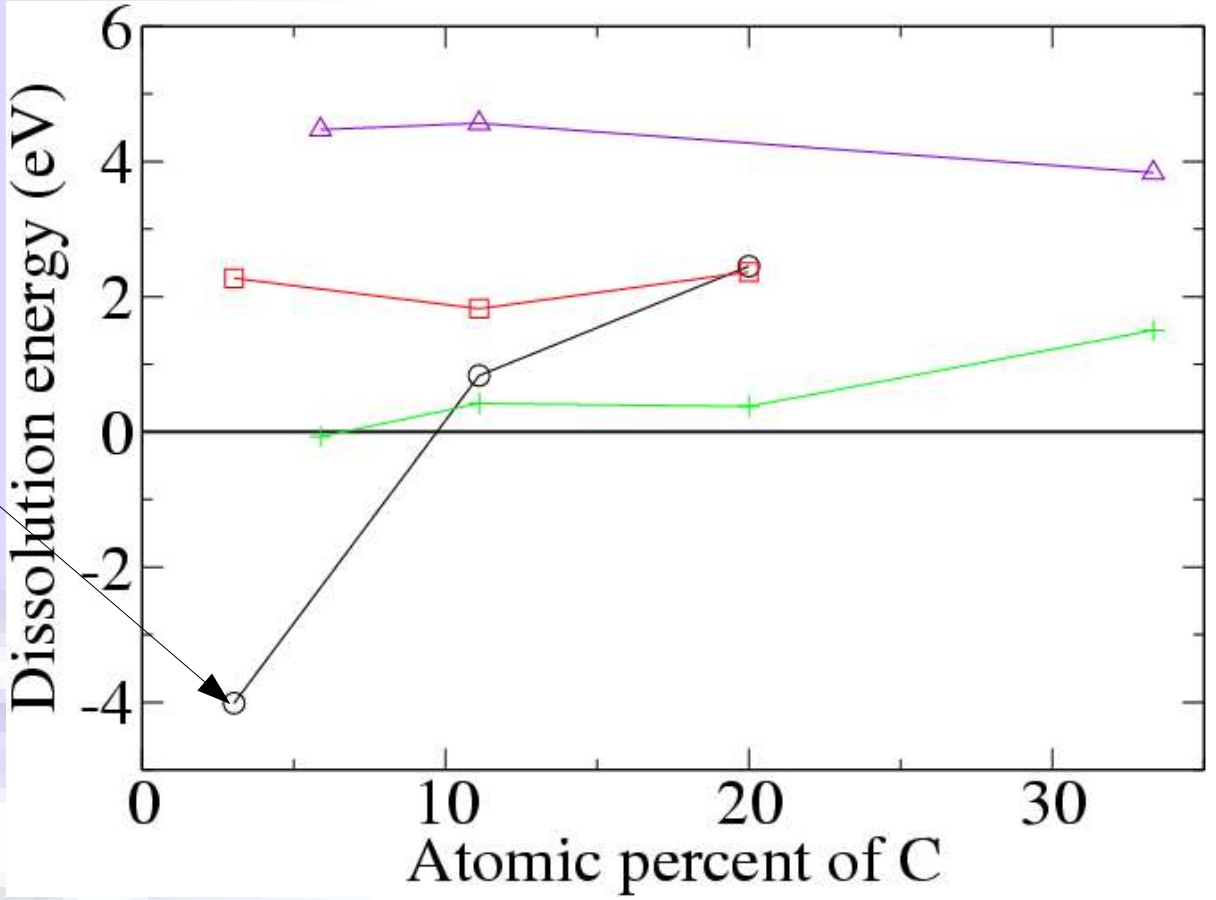




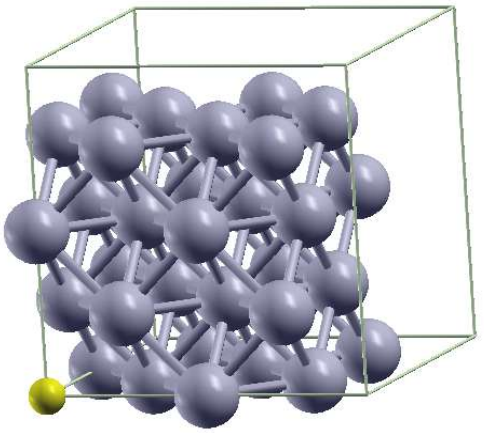


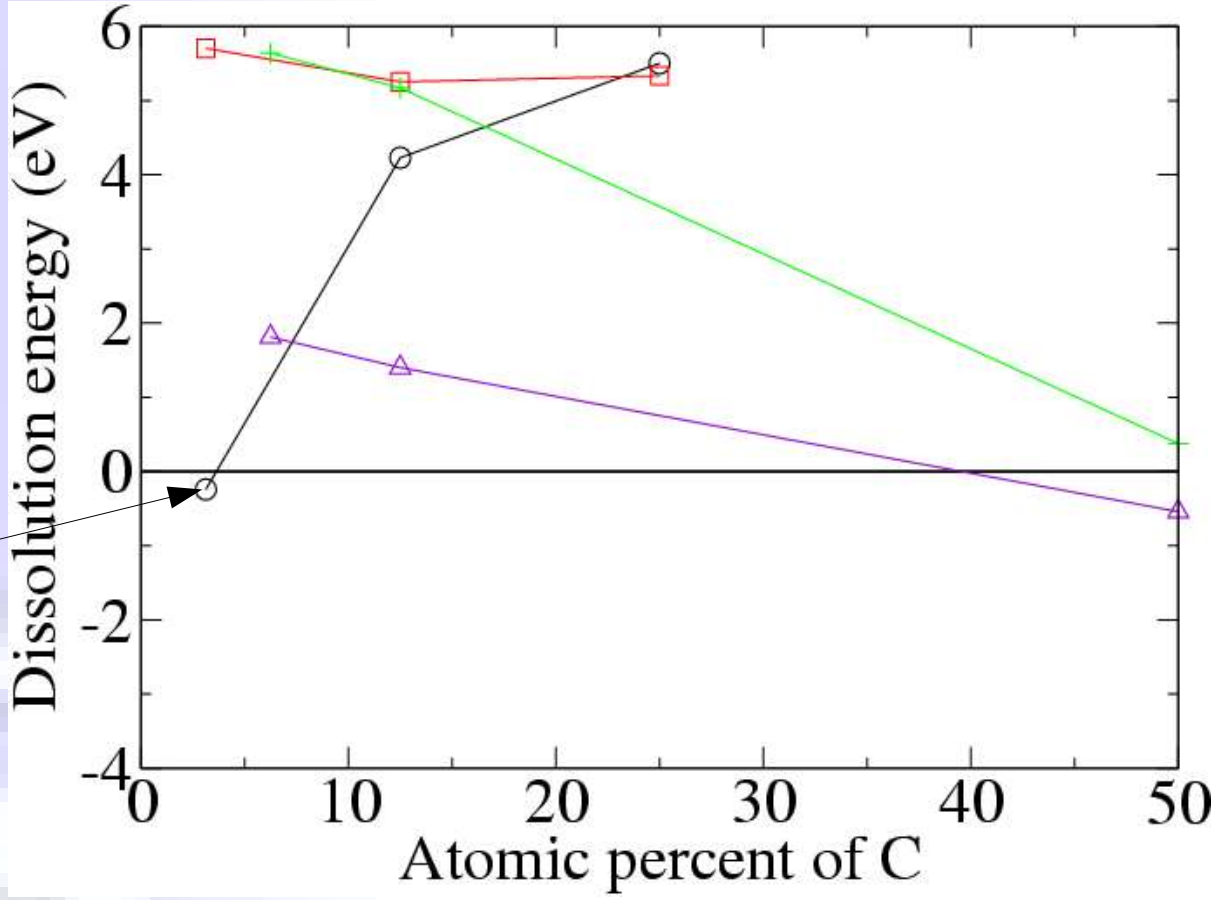
- Intf en: Ir(0.42) Pt(0.38) Si(0.36) Re(0.04) eV/Å^2
- Strains: Ir(7.8%) Pt(10.2%) Si(7.9%) Re(9.7%)
- Re is (111): compact plane can lower intf en
- Si is “mis-aligned” real value may be lower



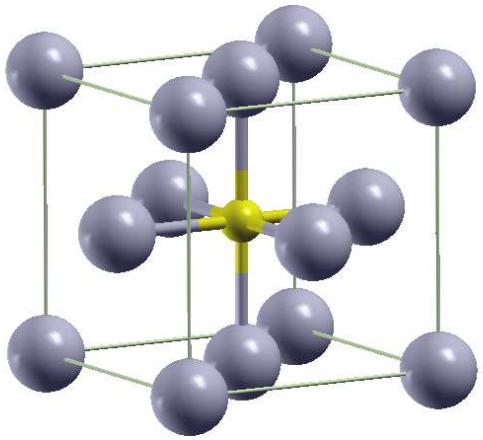


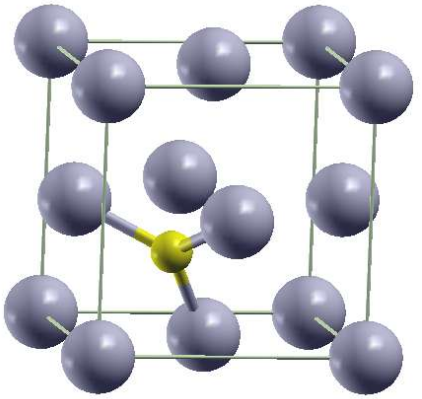
- Interface energies close (except Re (111)) So what?
- Interstitial dissolution in Ir is very favorable at low concentration

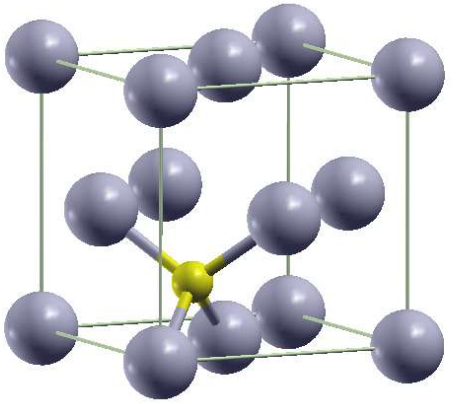




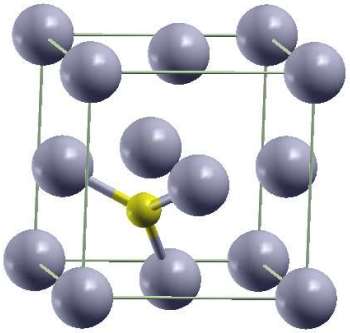
- Substitutional dissolution is less favorable
- Except for 50% concentration in Si (and Re) - carbides form

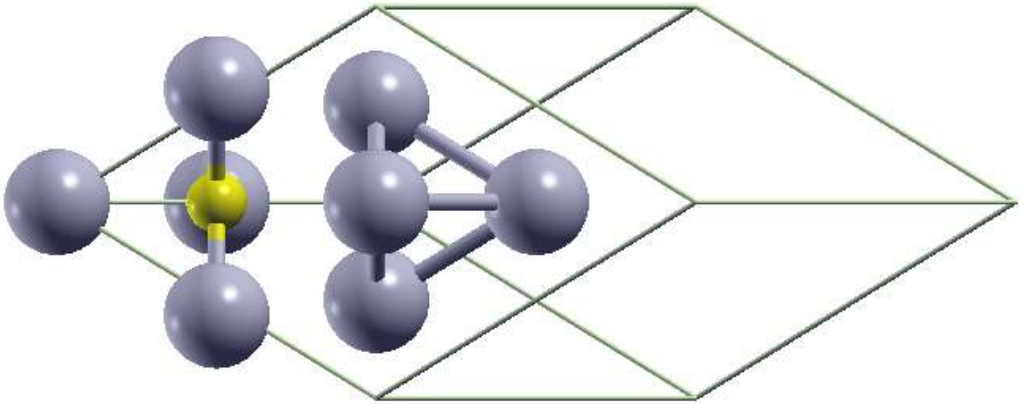




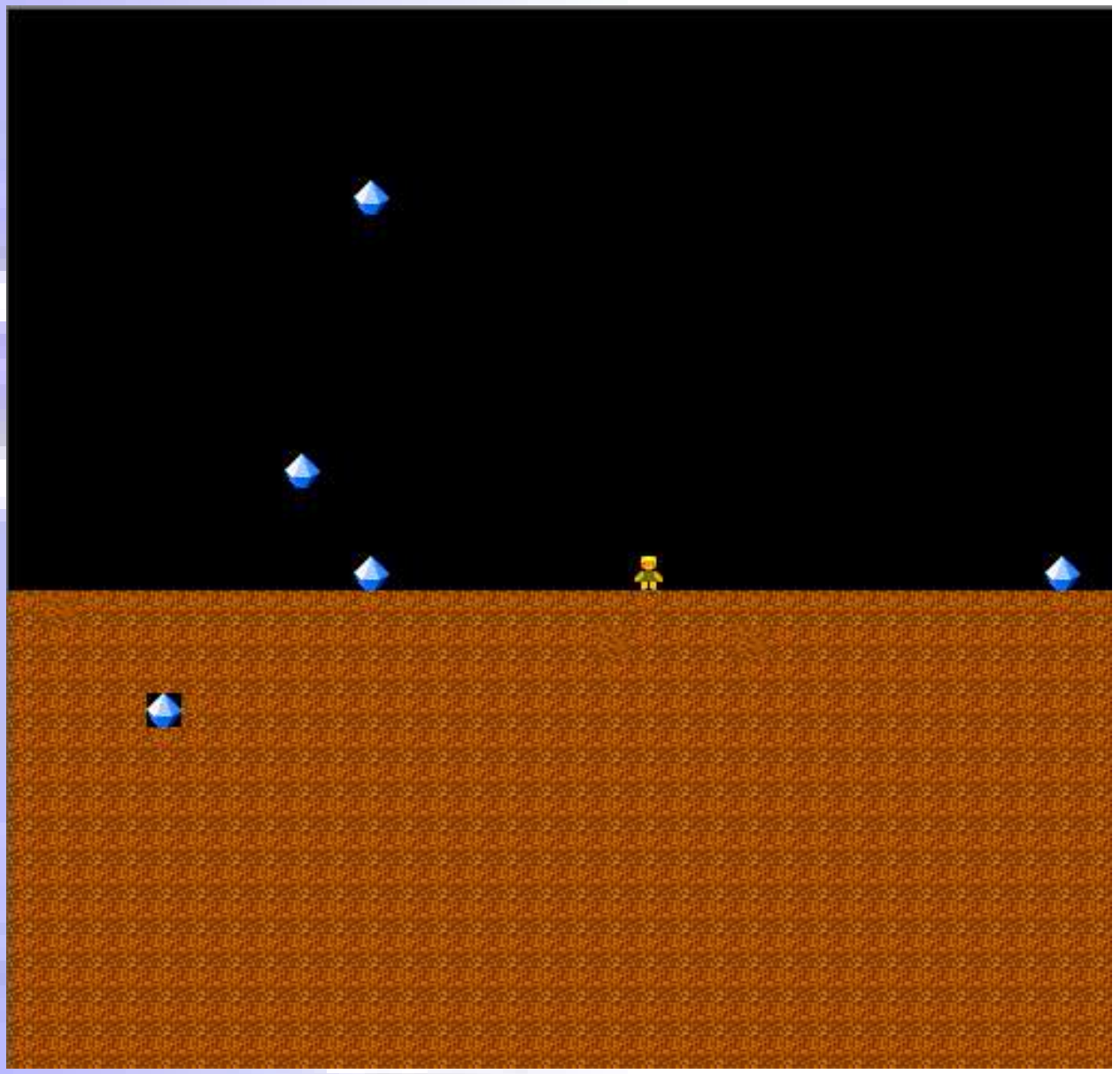


- Migration through octa → face → tetra → face → octa path
- Calculate upper bound for migration energy
- Fix cell size and relax atoms
- Octahedral face position must be constrained

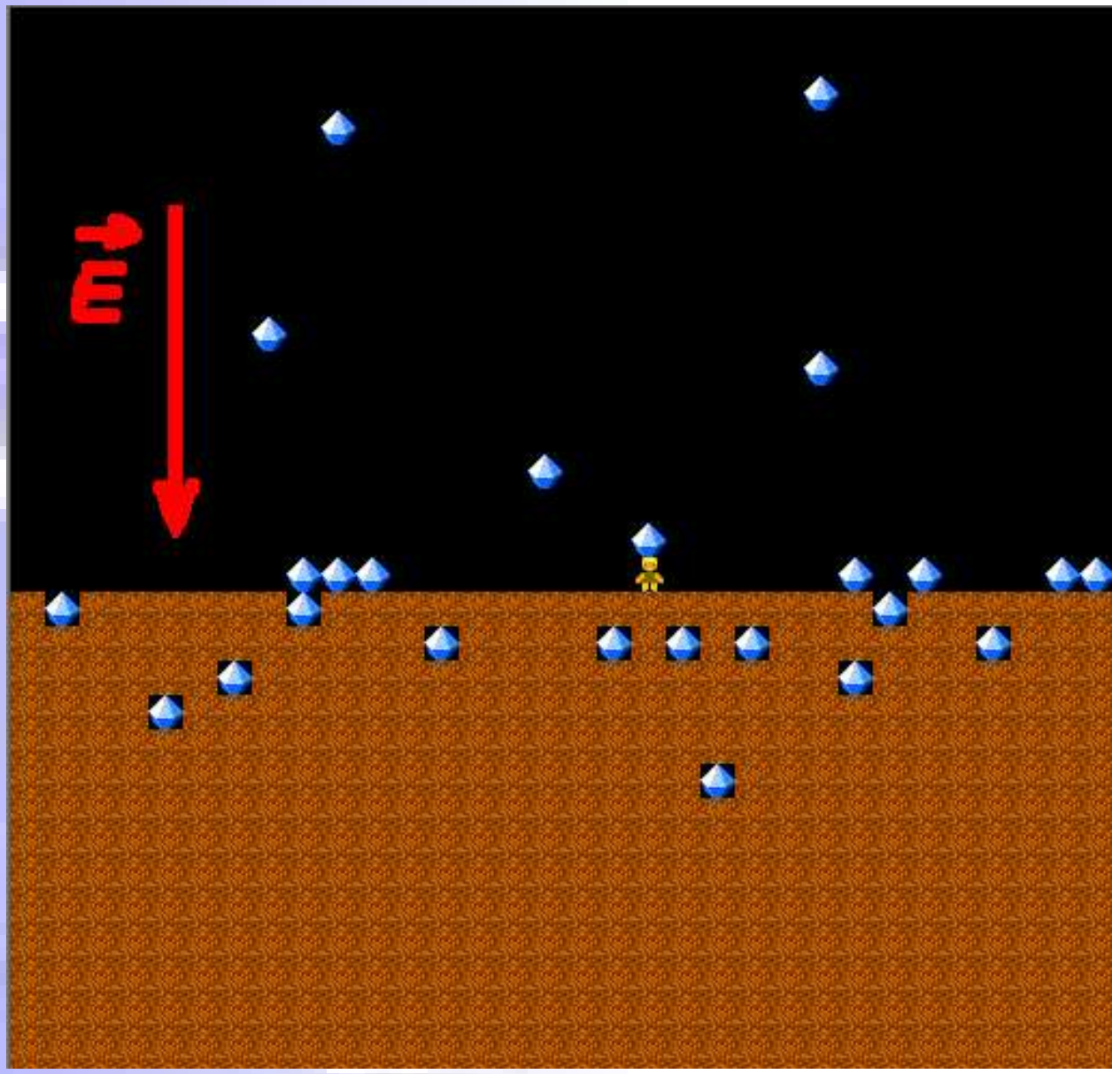




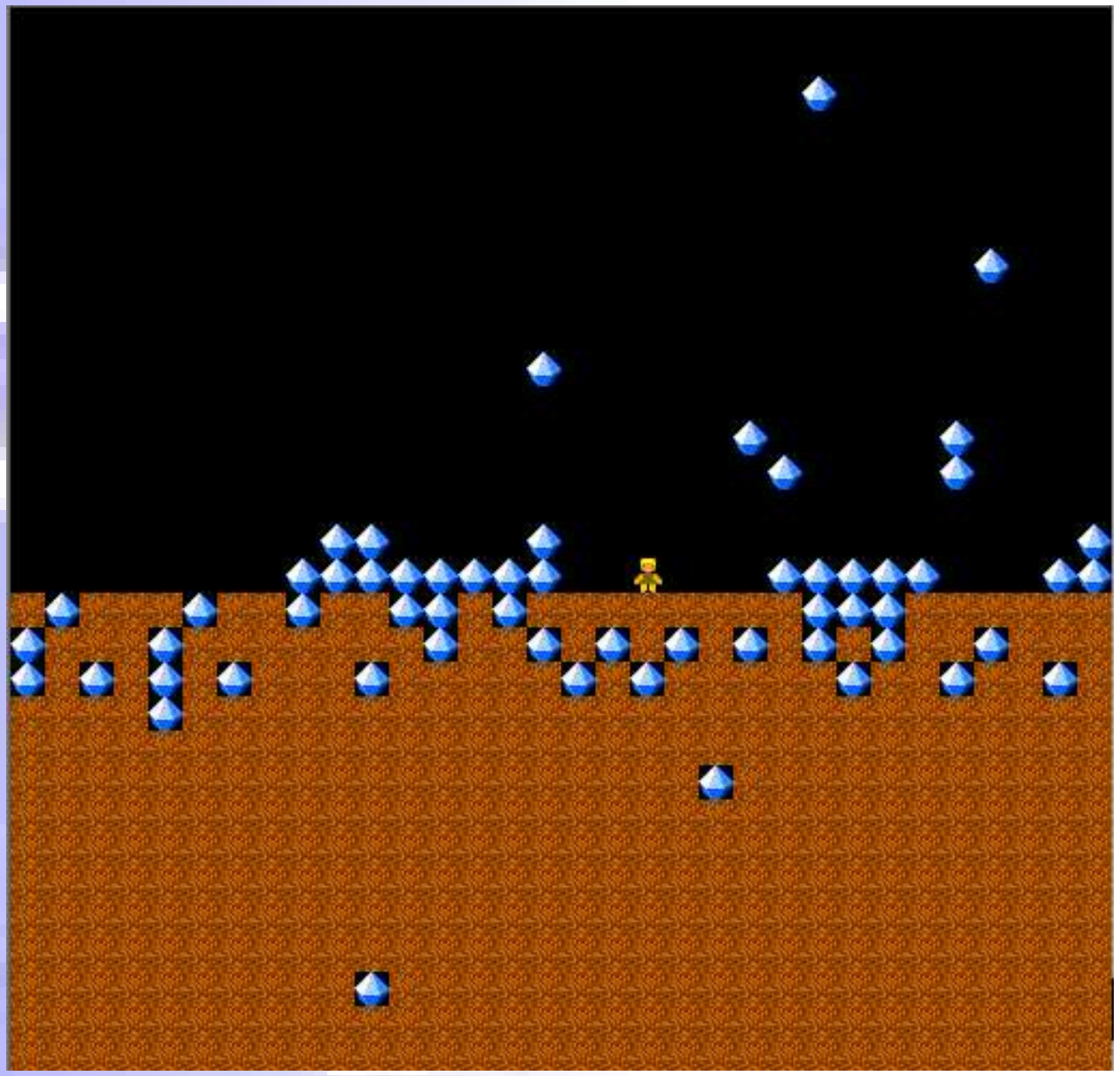
- Constrain positions of C and neighboring Ir along x only
- Orient 2x2x2 supercell appropriately
- Make a model...



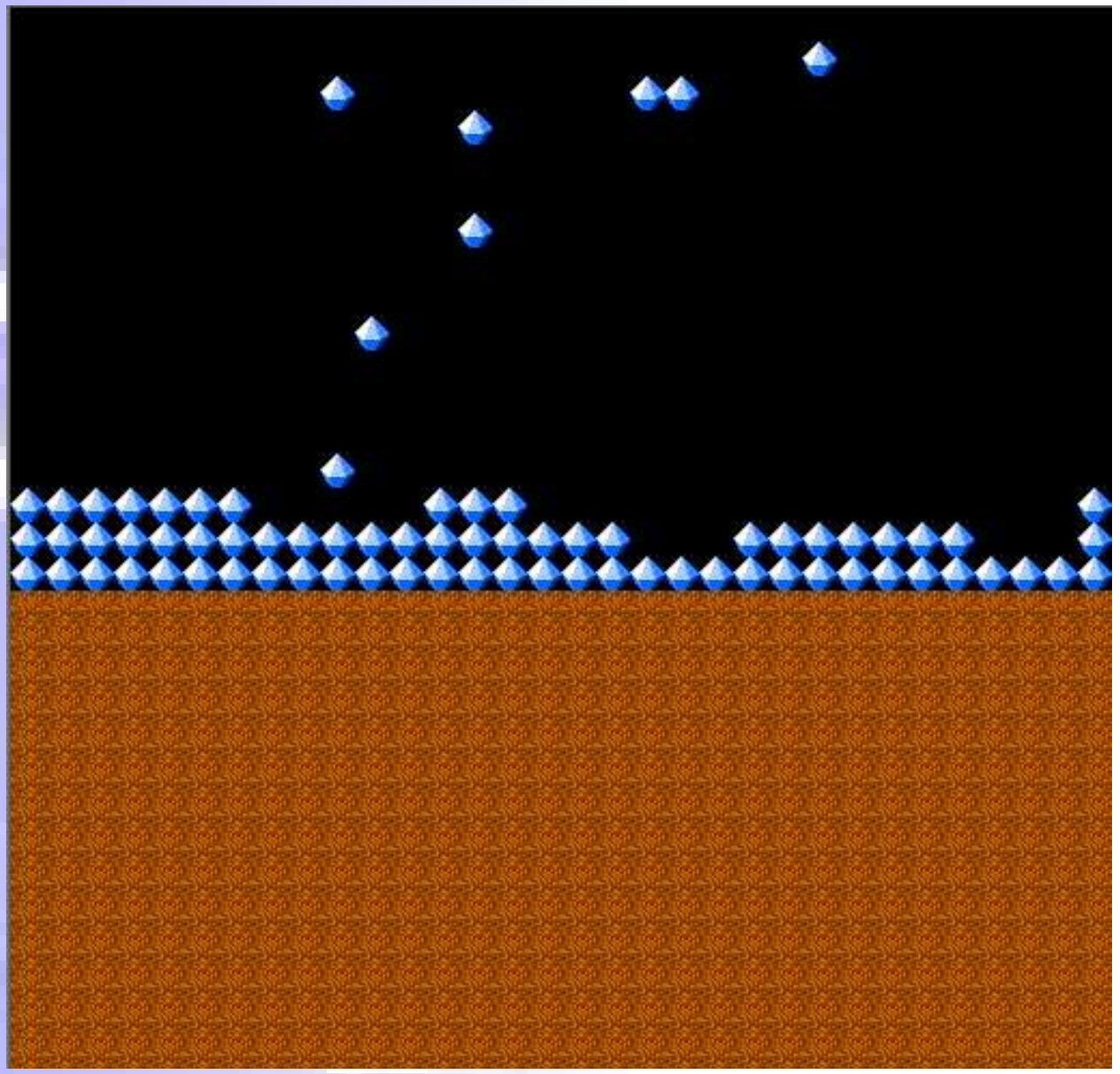
- CVD produces diamond films at low temperatures



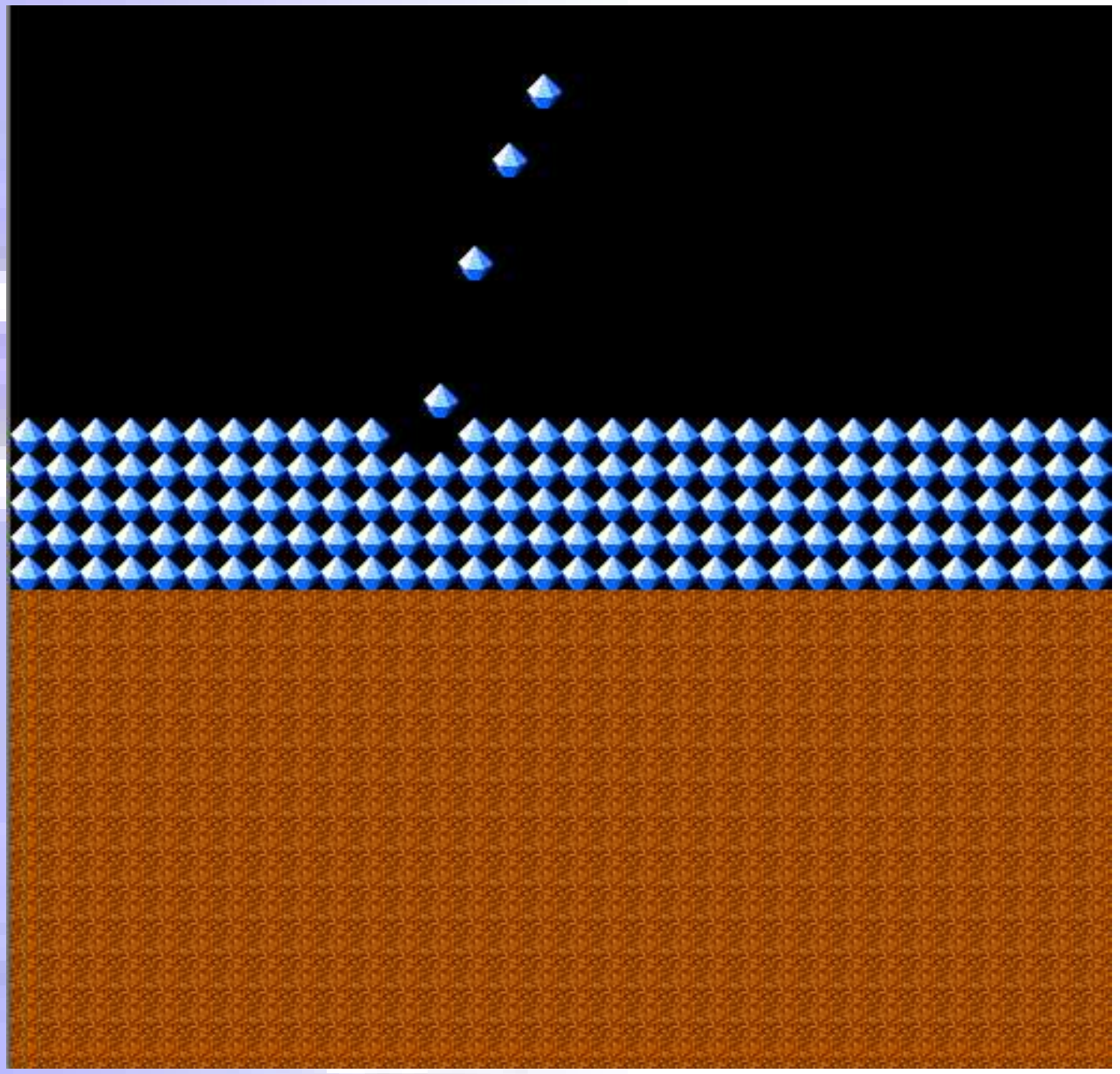
- Bias Enhanced Nucleation is necessary



- Improved nucleation (roughness, amount of C)



- Beyond 15% migration becomes possible and C is expelled



- The film grows on the nucleated monocrystalline islands

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Conclusions

- Qualitative difference for Ir is confirmed ab initio
- Surface energies don't count here
- Dissolution favored for low concentration → explain dynamics
- Find cheaper material with similar en vs. concentration profile