Void Swelling and Radiation-induced Segregation: An Example of the Need for Advances in Computational Modeling

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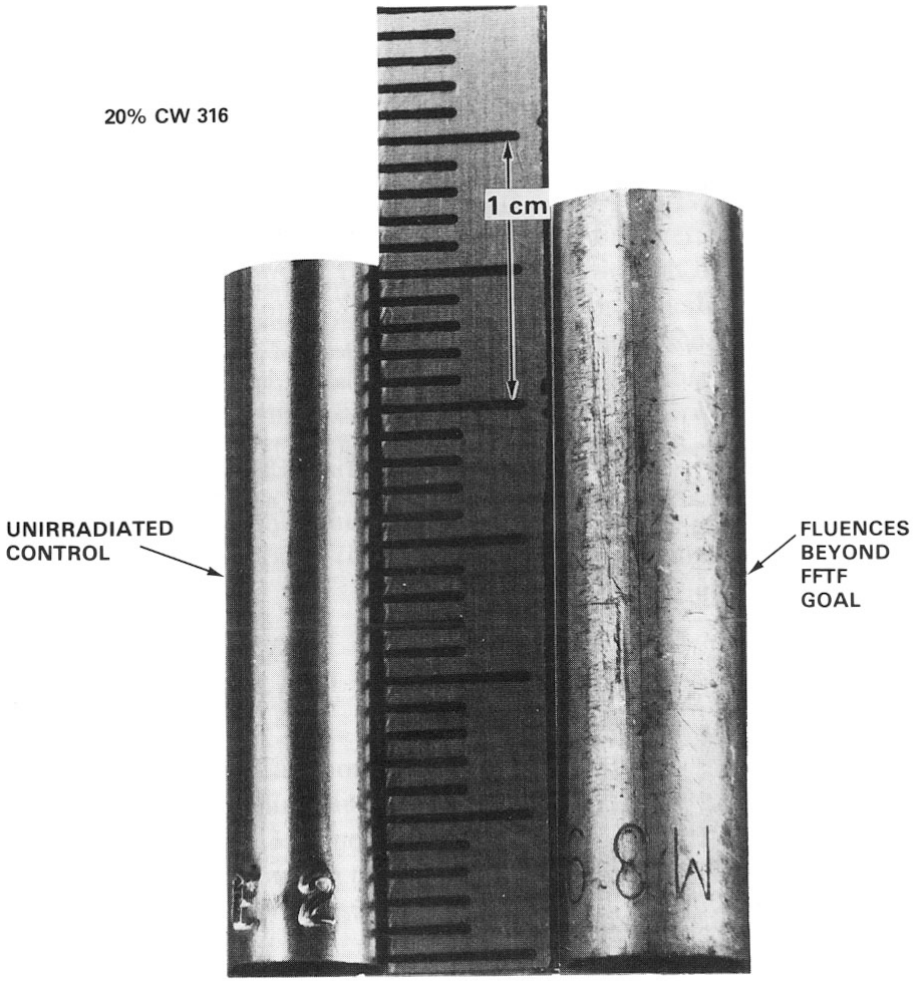
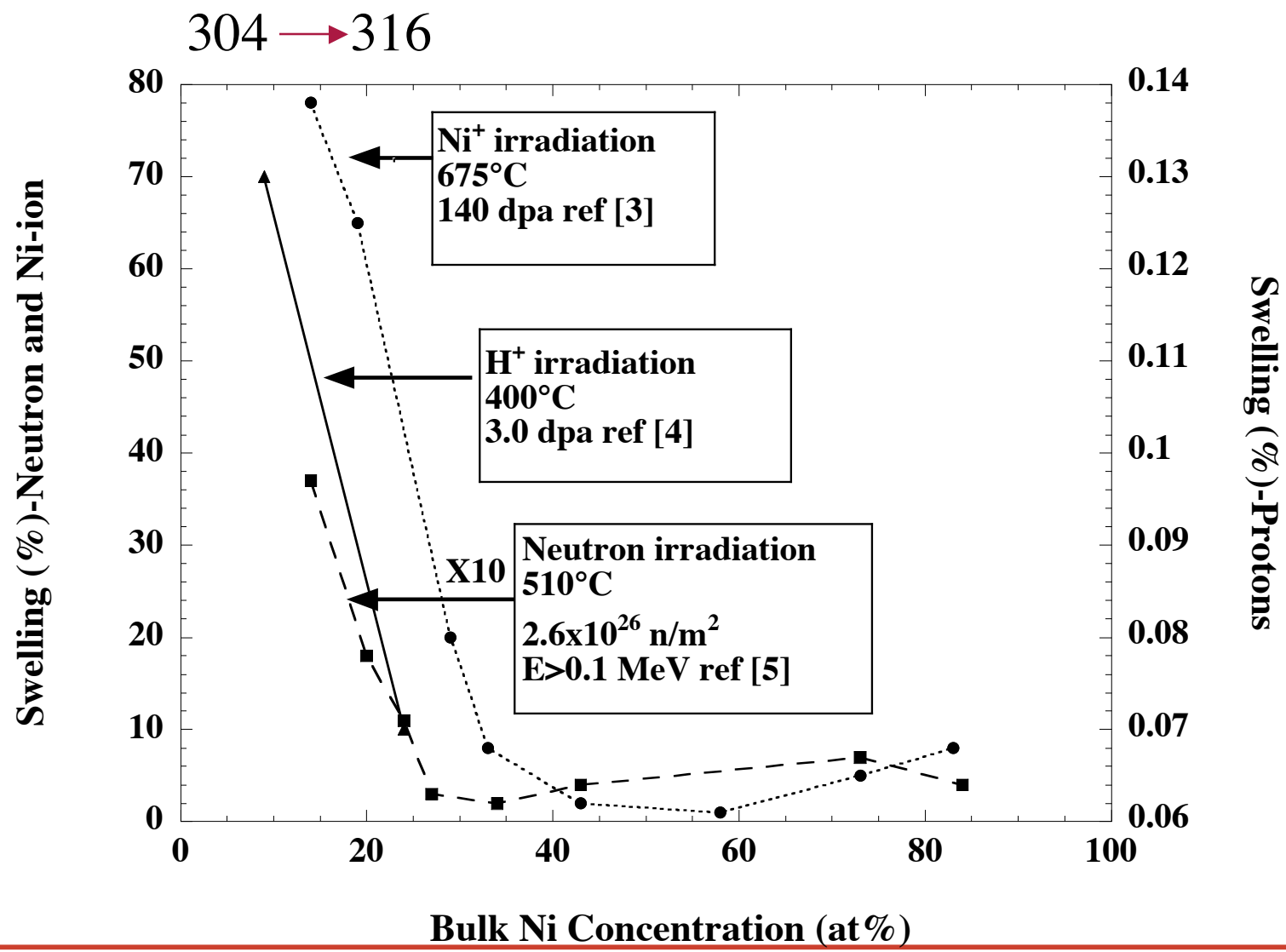
Easily Observed Swelling



- **Swelling: Volume increase in a material caused by void formation and growth**

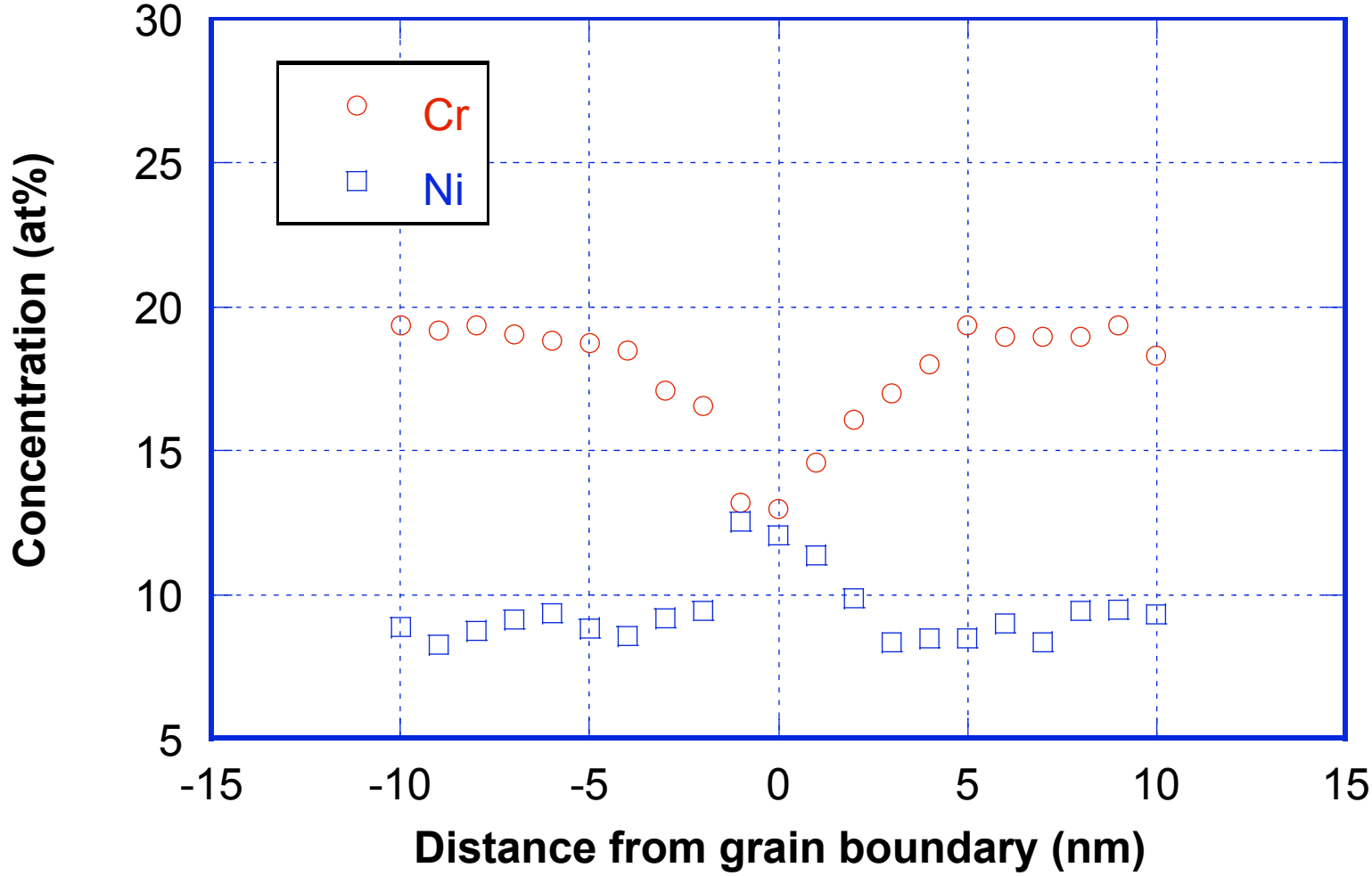
"The first open literature report of void formation during neutron irradiation sent a shock wave through the world's fast breeder reactor programs." (E. Bloom ASTM 2004 plenary talk)

Swelling and Bulk Composition



Grain Boundary Segregation

304 SS, proton irradiated at 400°C to a dose of 1.0 dpa



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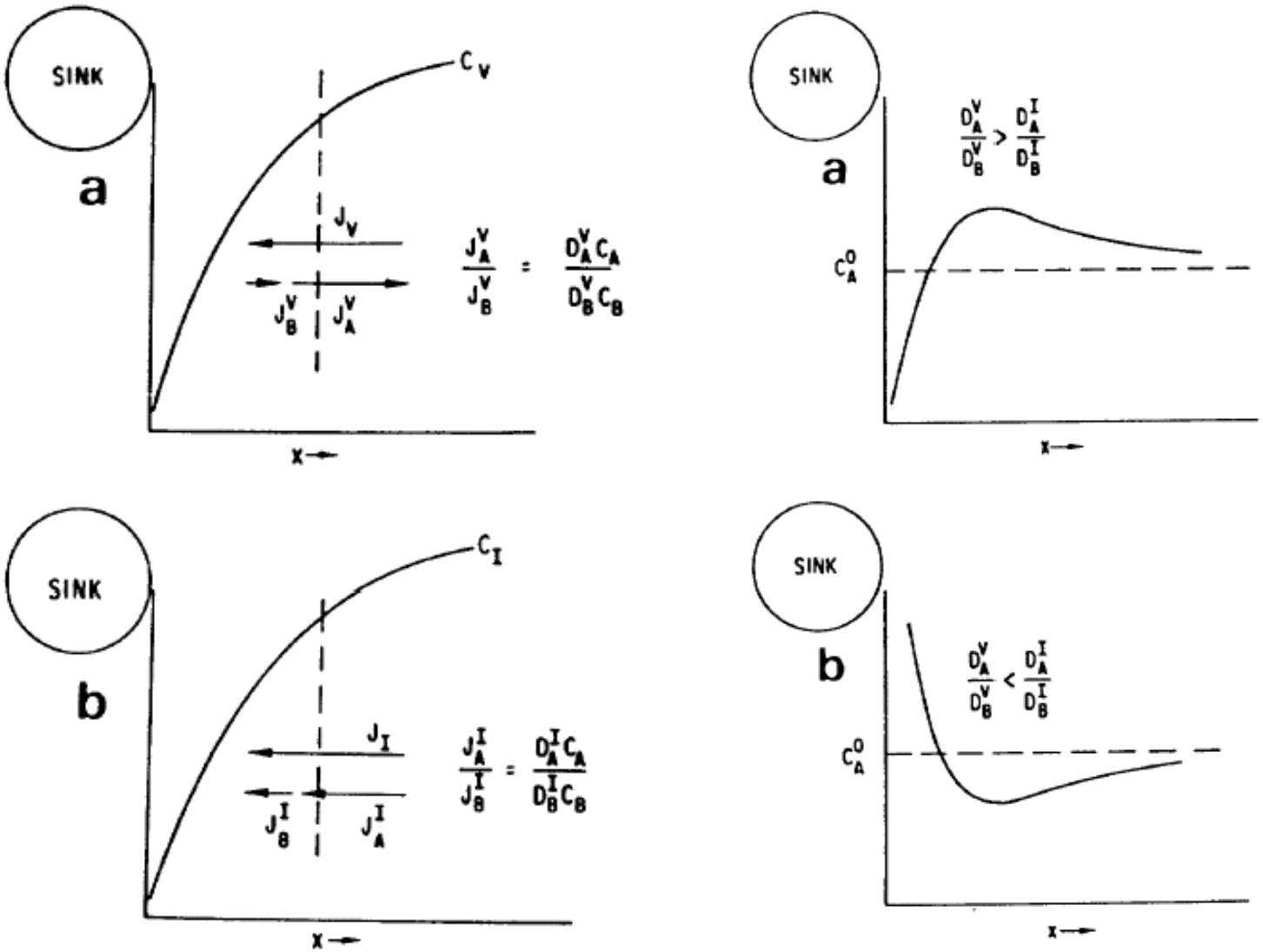


Segregation and Swelling

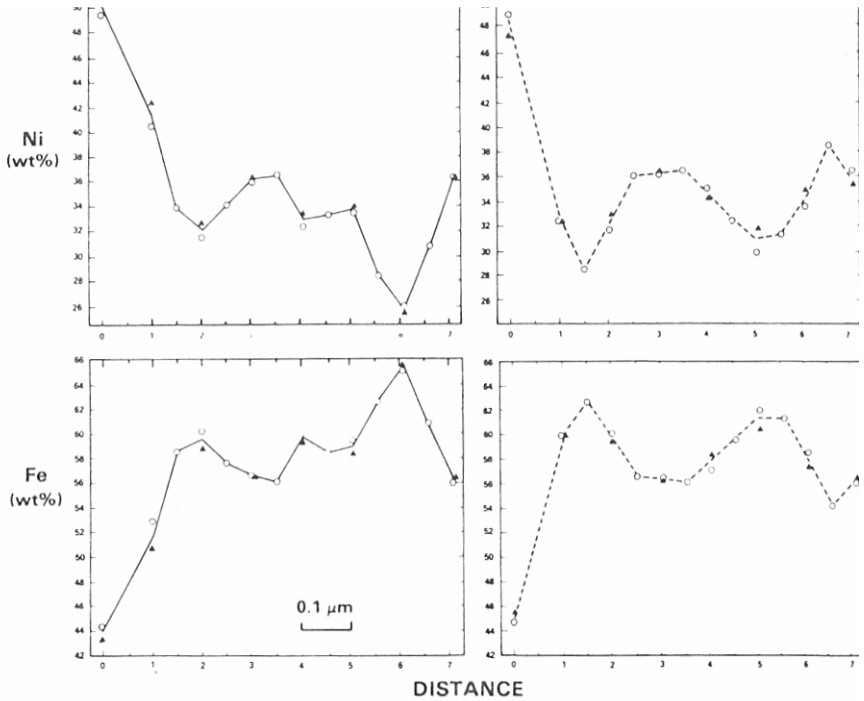


FIG. 8—*Compositional traverses starting from void or inclusion-precipitate markers. Note the reproducibility when measured twice on separate days.*

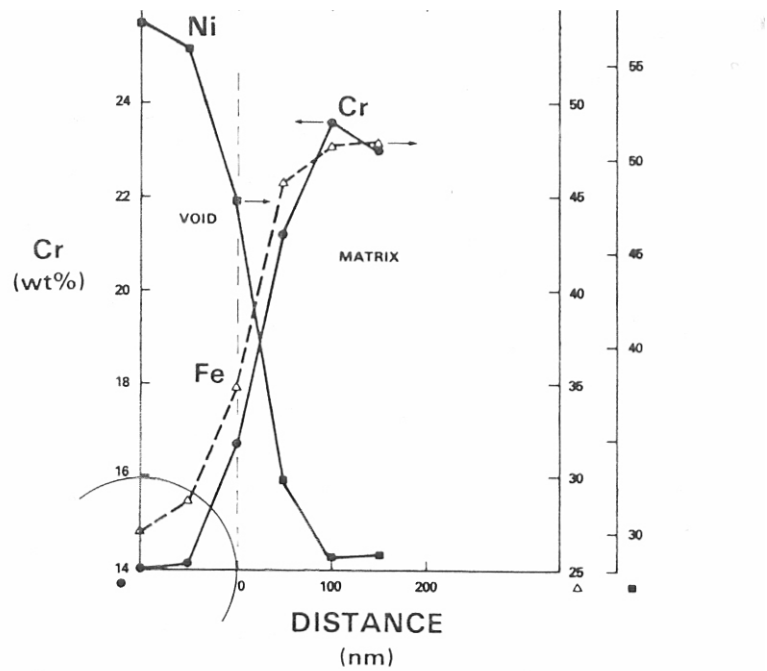
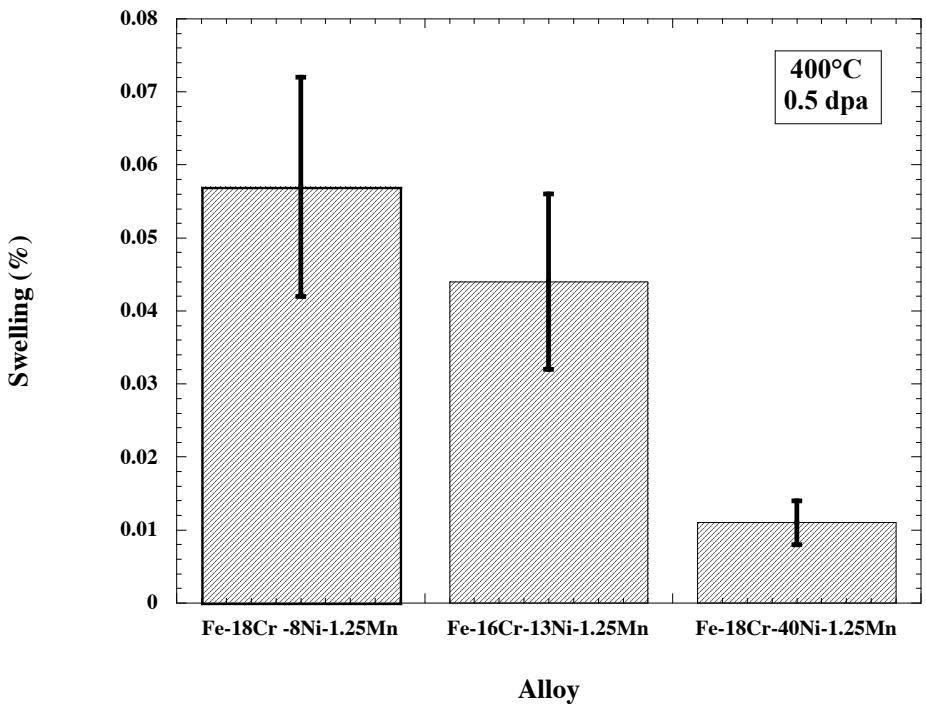
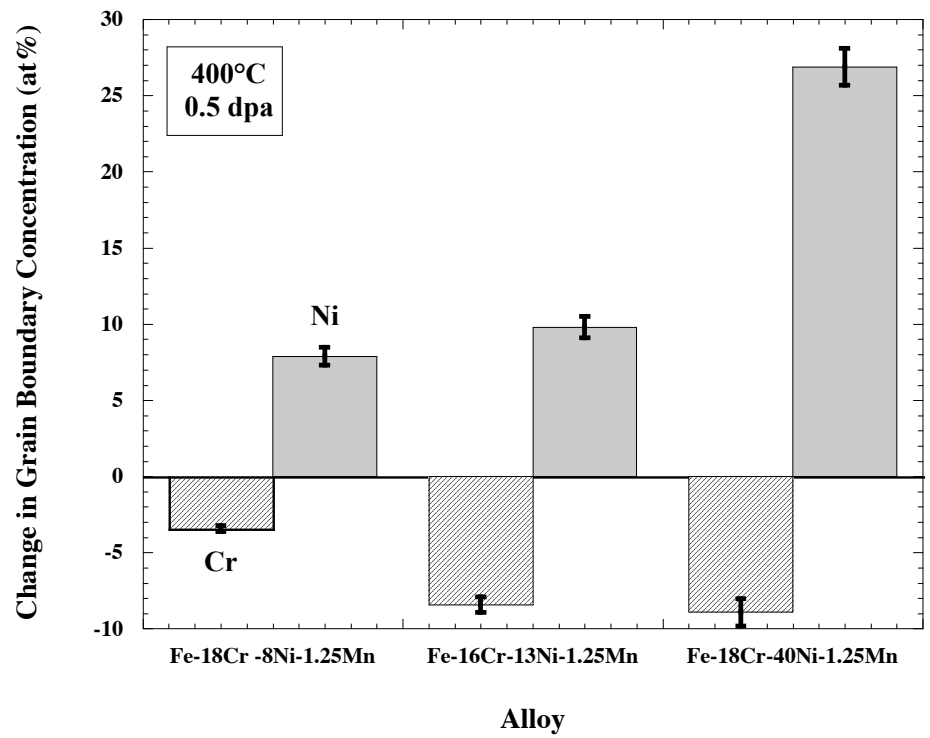


FIG. 11—*Concentration profiles observed in the vicinity of a void surface in Fe-35.1Ni-21.7Cr alloy irradiated to 7.2 × 10^{22} n/cm^2 (E > 0.1 MeV) at 538°C.* [21]. *Note the reduction in matrix nickel content due to segregation at the void surfaces.*

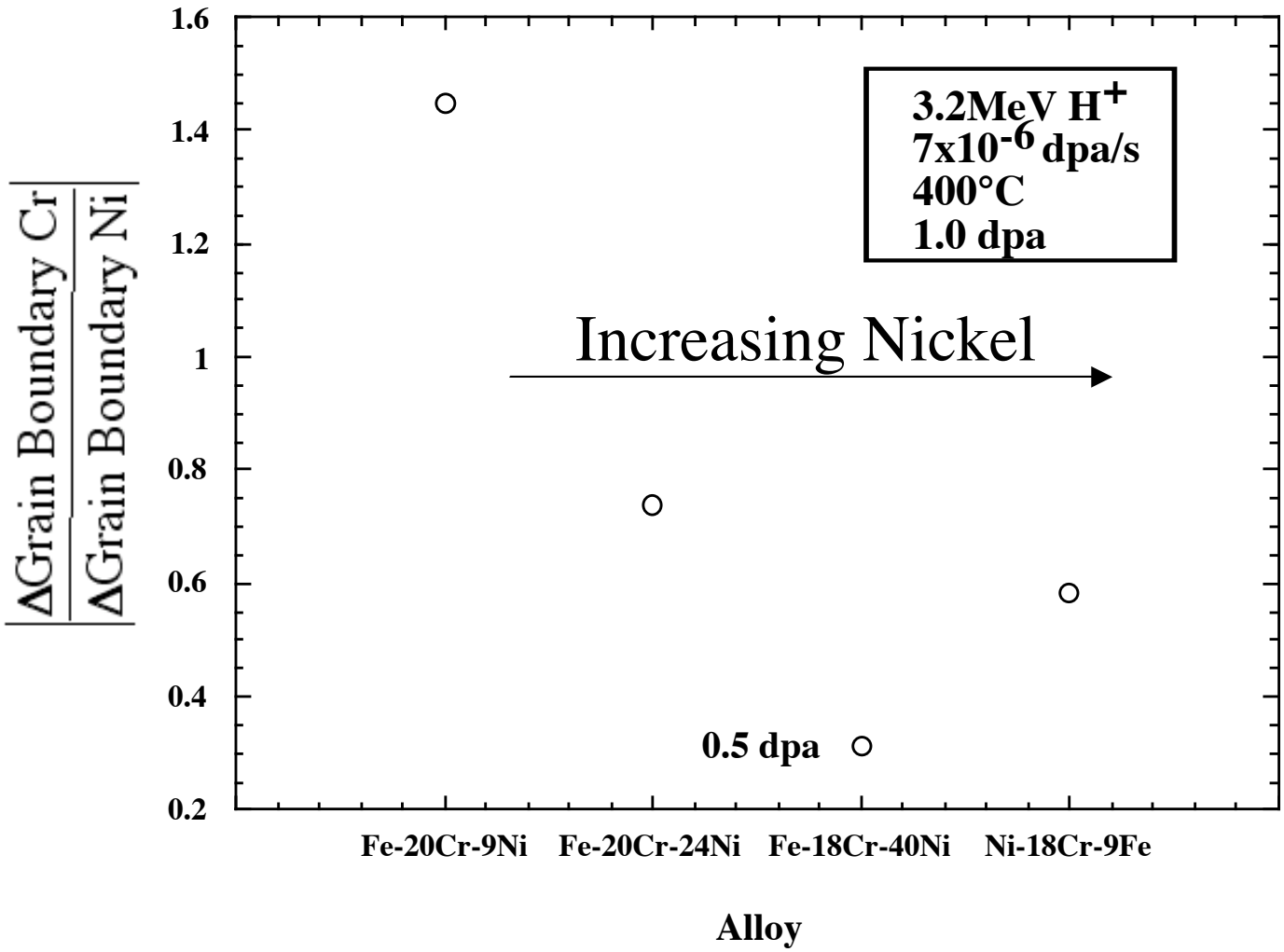
Brager and Garner

Segregation and Swelling

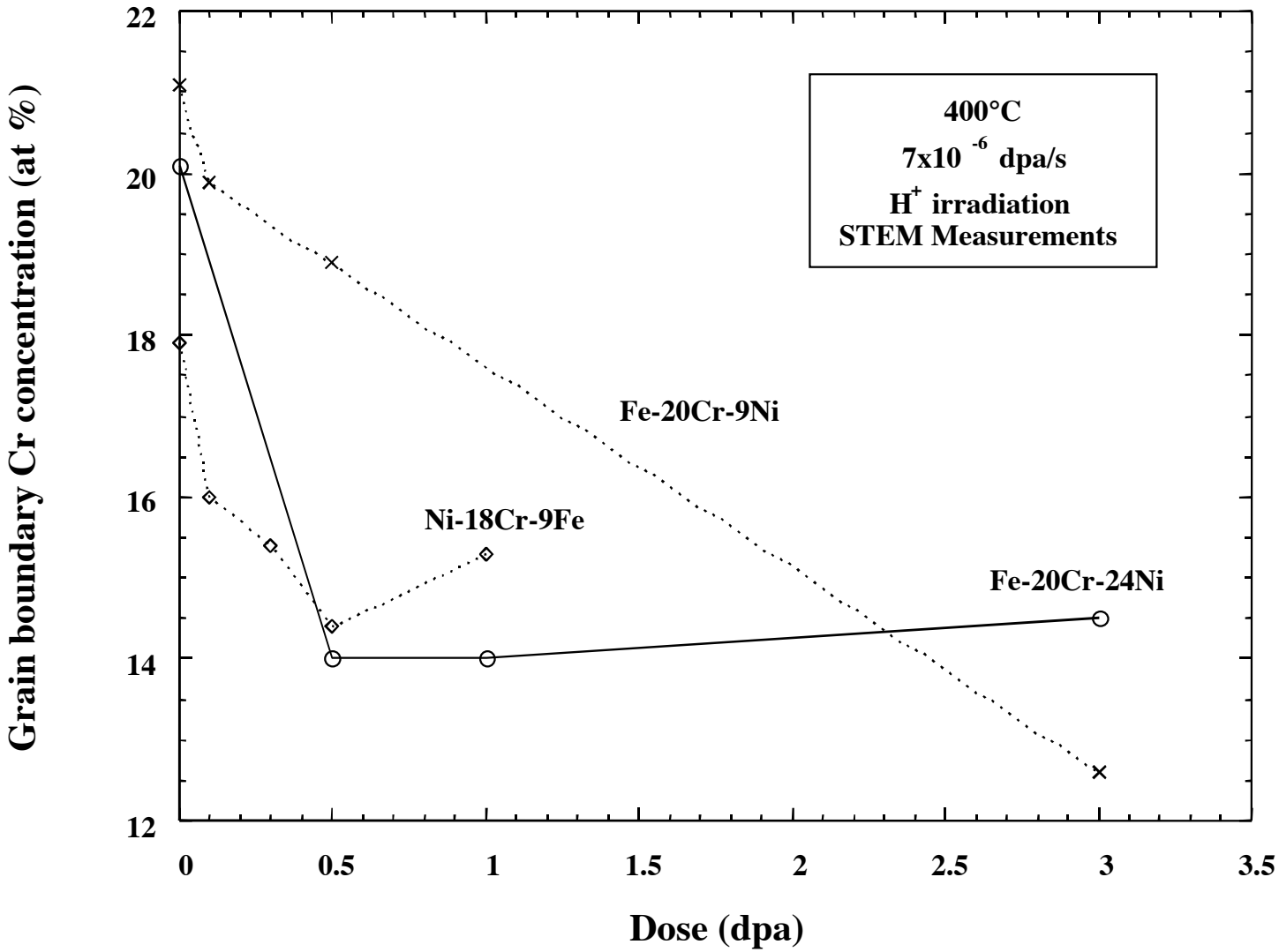




Segregation and Bulk Composition

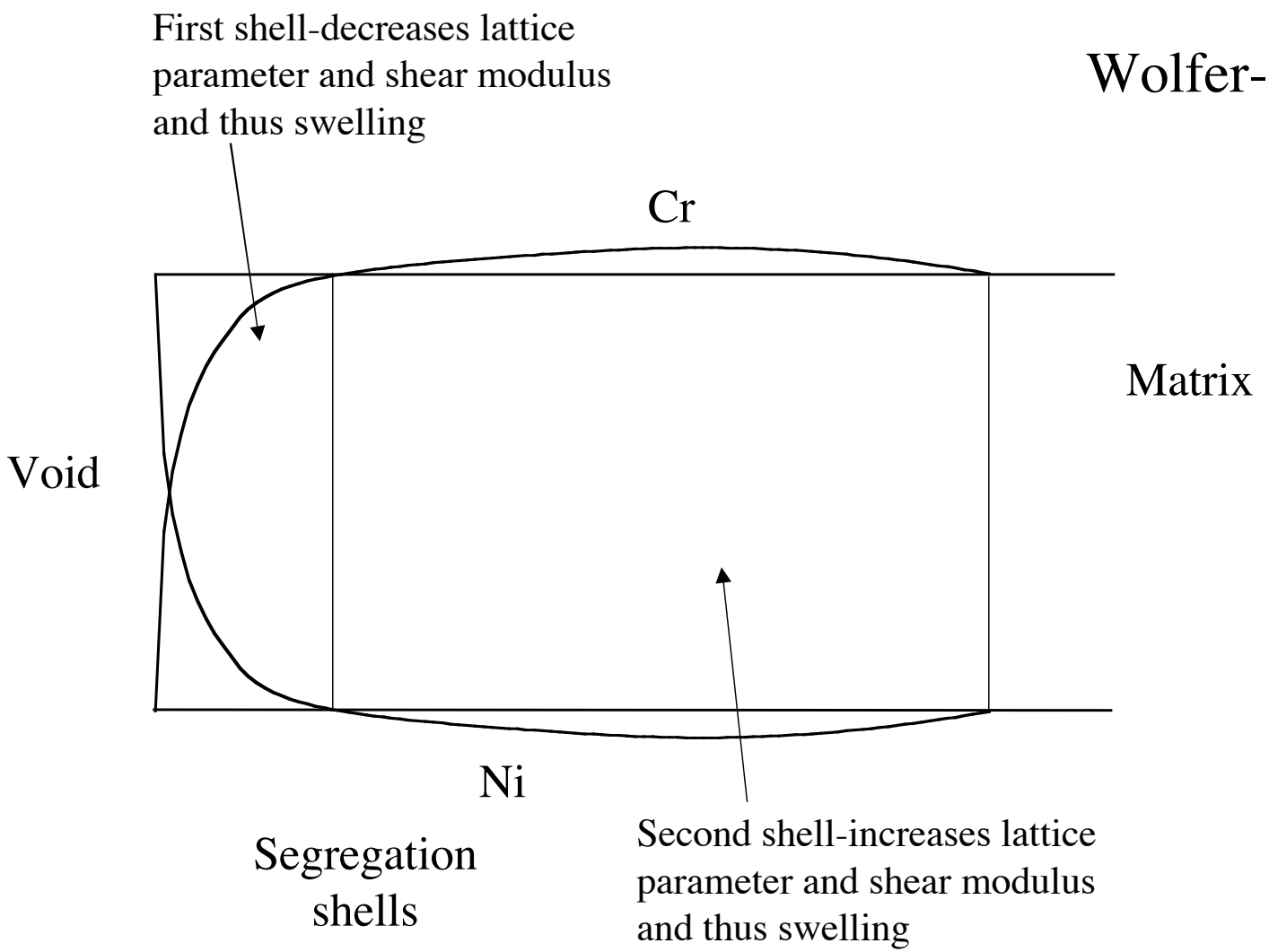


Segregation and Bulk Composition

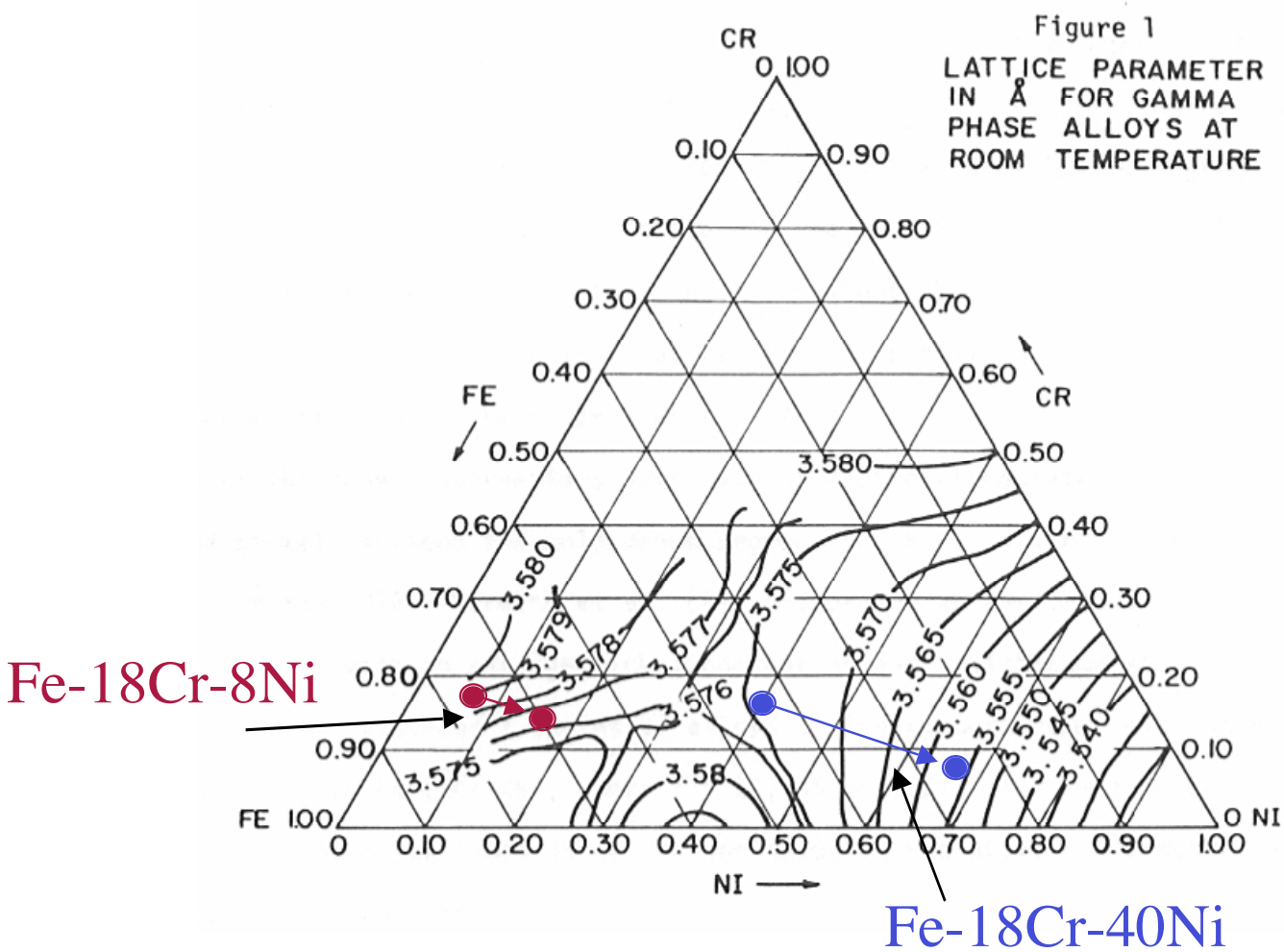


RIS and Void Bias

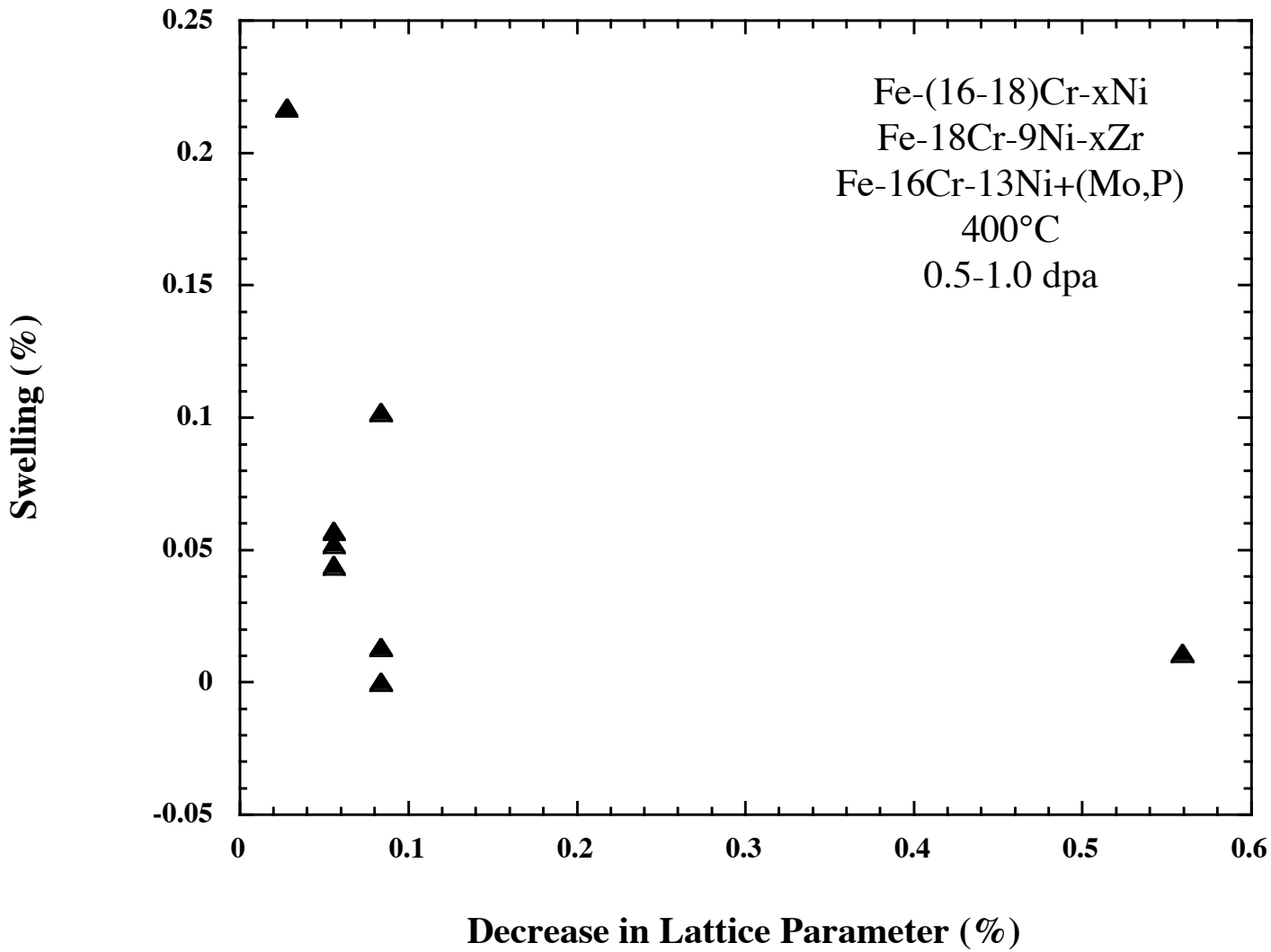
Wolfer-1970s



RIS and Lattice Parameter



RIS and Lattice Parameter



Key insight

Accurate modeling of radiation induced microstructural development requires the ability to model microchemical changes in complex alloys

Modeling Radiation Induced Segregation

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A system of four coupled partial differential equations describing the space and time dependence of the atoms and defects in the solid is determined by substituting the defect and atom fluxes given by eqns (11) into eqns (1) and (5):

$$\frac{\partial C_v}{\partial t} = \nabla \bullet [-(d_{Av} - d_{Cv})\Omega C_v \alpha \nabla C_A - (d_{Bv} - d_{Cv})\Omega C_v \alpha \nabla C_B + D_v \nabla C_v] + K - R, \quad (13a)$$

$$\frac{\partial C_i}{\partial t} = \nabla \bullet [(d_{Ai} - d_{Ci})\Omega C_i \alpha \nabla C_A + (d_{Bi} - d_{Ci})\Omega C_i \alpha \nabla C_B + D_i \nabla C_i] + K - R, \quad (13b)$$

$$\frac{\partial C_A}{\partial t} = \nabla \bullet [D_A \alpha \nabla C_A + \Omega C_A (d_{Ai} \nabla C_i - d_{Av} \nabla C_v)], \quad (13c)$$

$$\frac{\partial C_B}{\partial t} = \nabla \bullet [D_B \alpha \nabla C_B + \Omega C_B (d_{Bi} \nabla C_i - d_{Bv} \nabla C_v)]. \quad (13d)$$

Calculations are made by equating a grain boundary to a free surface.

Initial conditions:

- thermodynamic equilibrium
- Atom concentrations are spatially uniform

Boundary conditions:

- $\nabla C_x(0,t) = 0$
- $C_{v,i}(0,t) = C_{v,i}^{eq}$

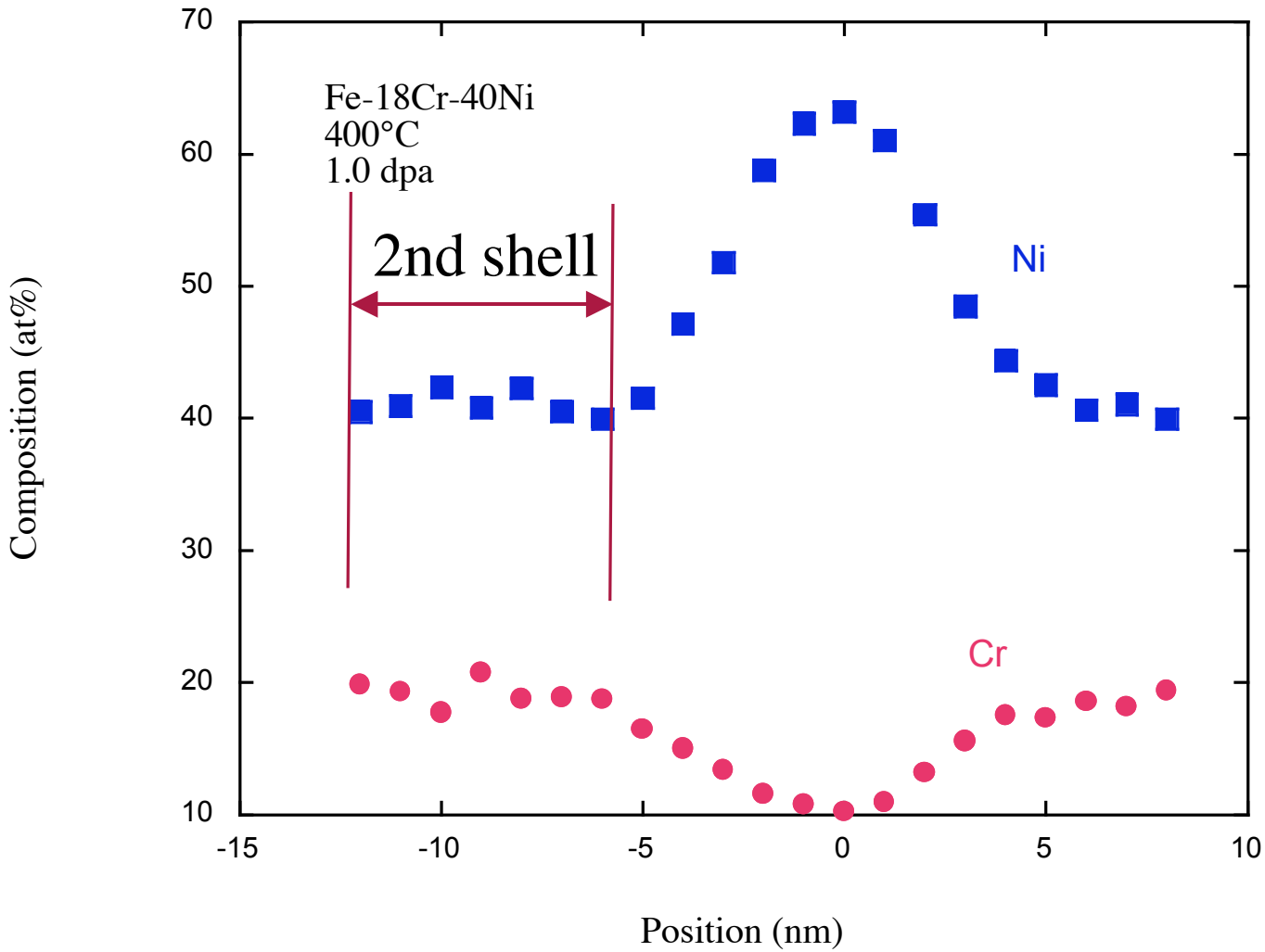
Data limitations

- Vacancy diffusion information must be extrapolated well beyond the experimental temperatures and into temperature regions where different phases are thermodynamically stable
- Uncertainties in vacancy diffusion data used in Arhennius expressions are "magnified" at low temperature
- Interstitial diffusion information for individual species is non-existent

Similar effects are expected for other key material properties

Conclusions

Computational modeling can provide key insights required to understand the complexity that drives microstructural development in engineering alloys

Backups

Second Shell