

*Welcome to 3.091*

Lecture 19

October 23, 2009

Point & Line Defects

# **Taxonomy of Defects:** **Classify by Dimensionality**

*0-dimensional:* point defects

*1-dimensional:* line defects

*2-dimensional:* interfacial defects

*3-dimensional:* bulk defects

## Point Defects

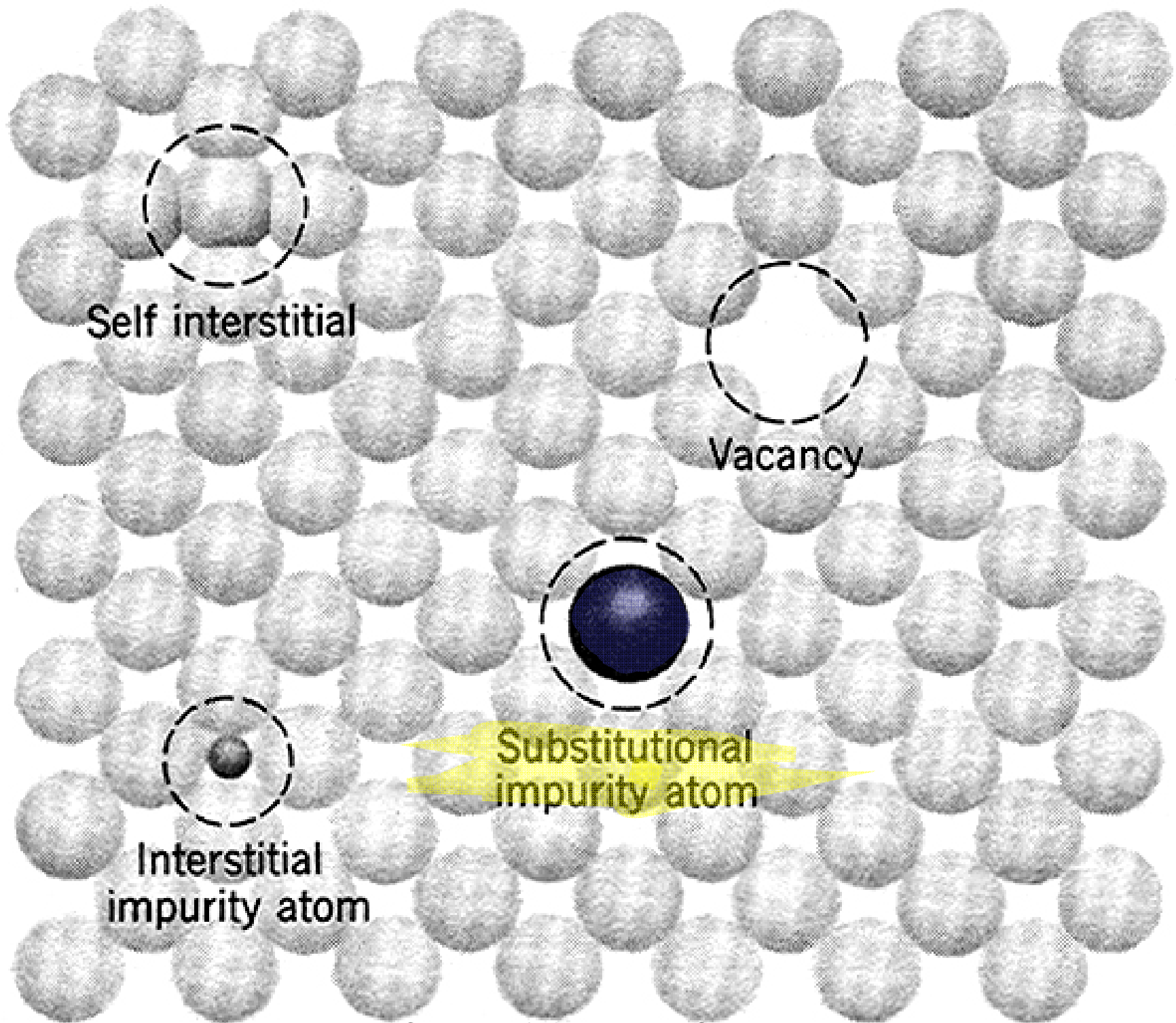
- localized disruption in regularity of the lattice
- on and between lattice sites

### 1. Substitutional Impurity

- occupies normal lattice site
- dopant ☺, e.g., P in Si; B in C<sub>(diamond)</sub>
- alloying element ☺, e.g., Mg in Al; or Ni in Au
- contaminant ☹, Li<sup>+</sup> in NaCl

### 2. Interstitial Impurity

- occupies position between lattice sites
- alloying element ☺, e.g., C in Fe; or H in LaNi<sub>5</sub>
- contaminant ☹, H in Fe



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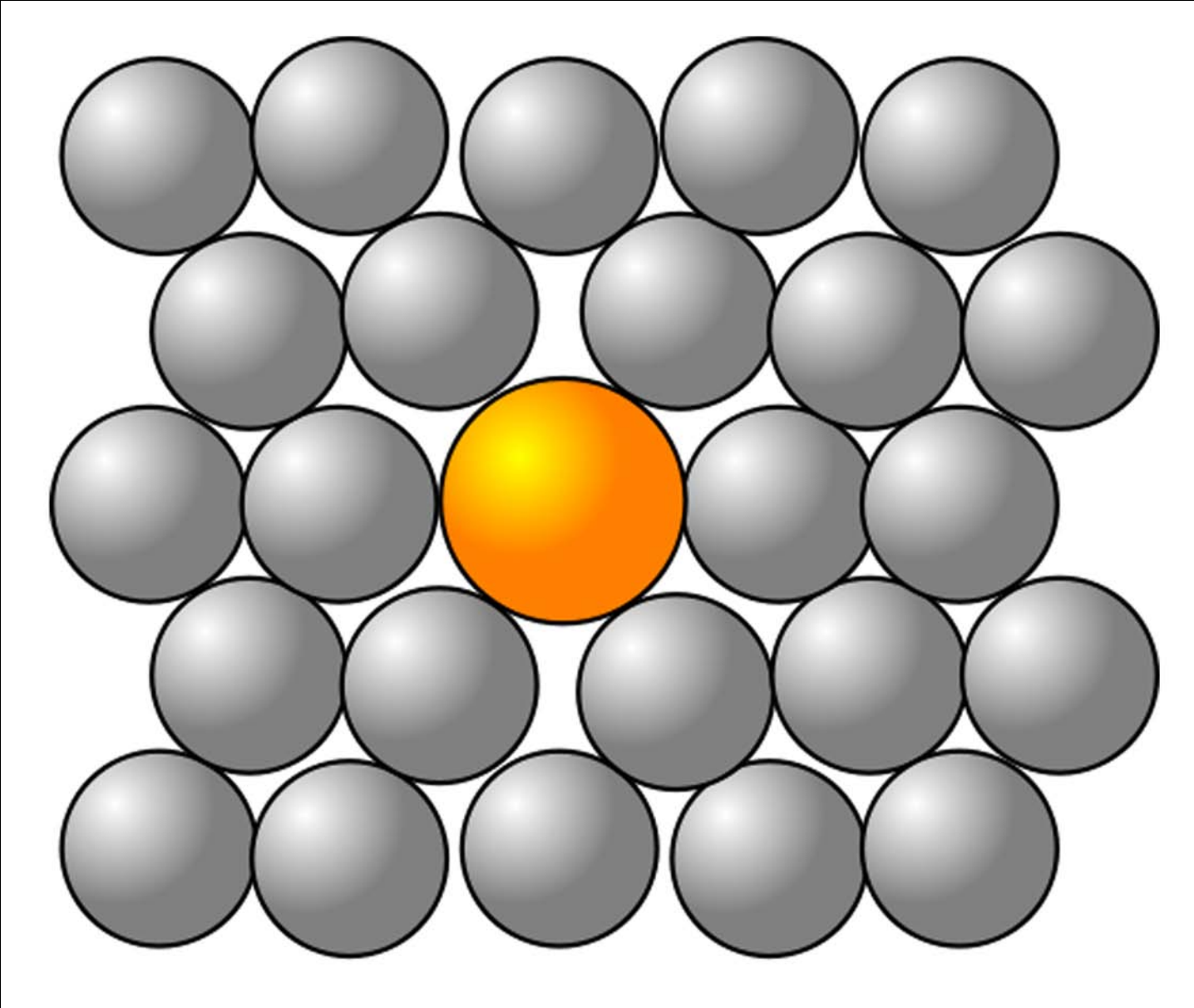


Image by [Cdang](#) on Wikipedia.

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Image removed due to copyright restrictions. Please see the cover of Post, Jeffrey E. *The National Gem Collection*. Washington, DC: Smithsonian Institution, 1997. ISBN: 9780810936904.



## Point Defects

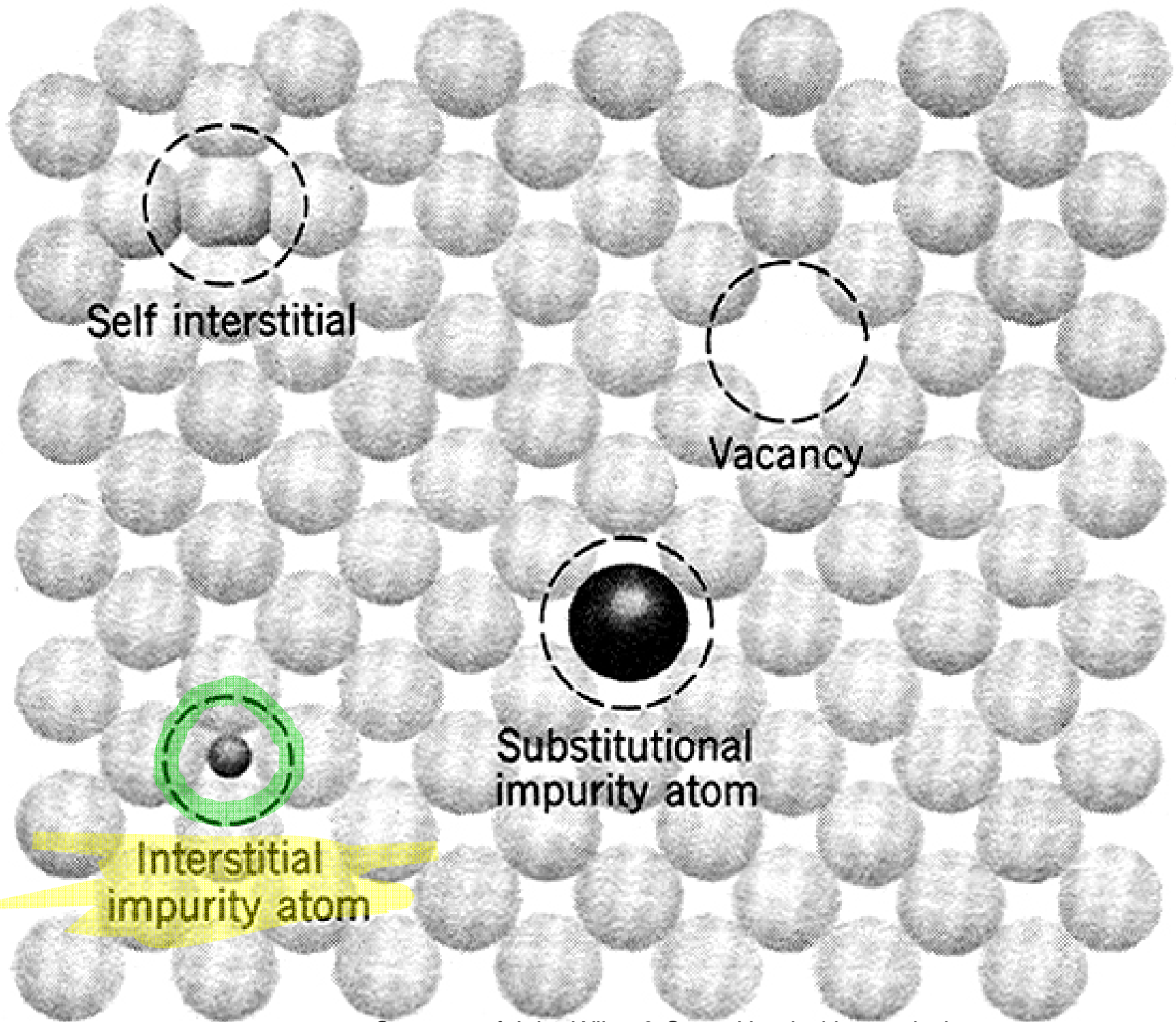
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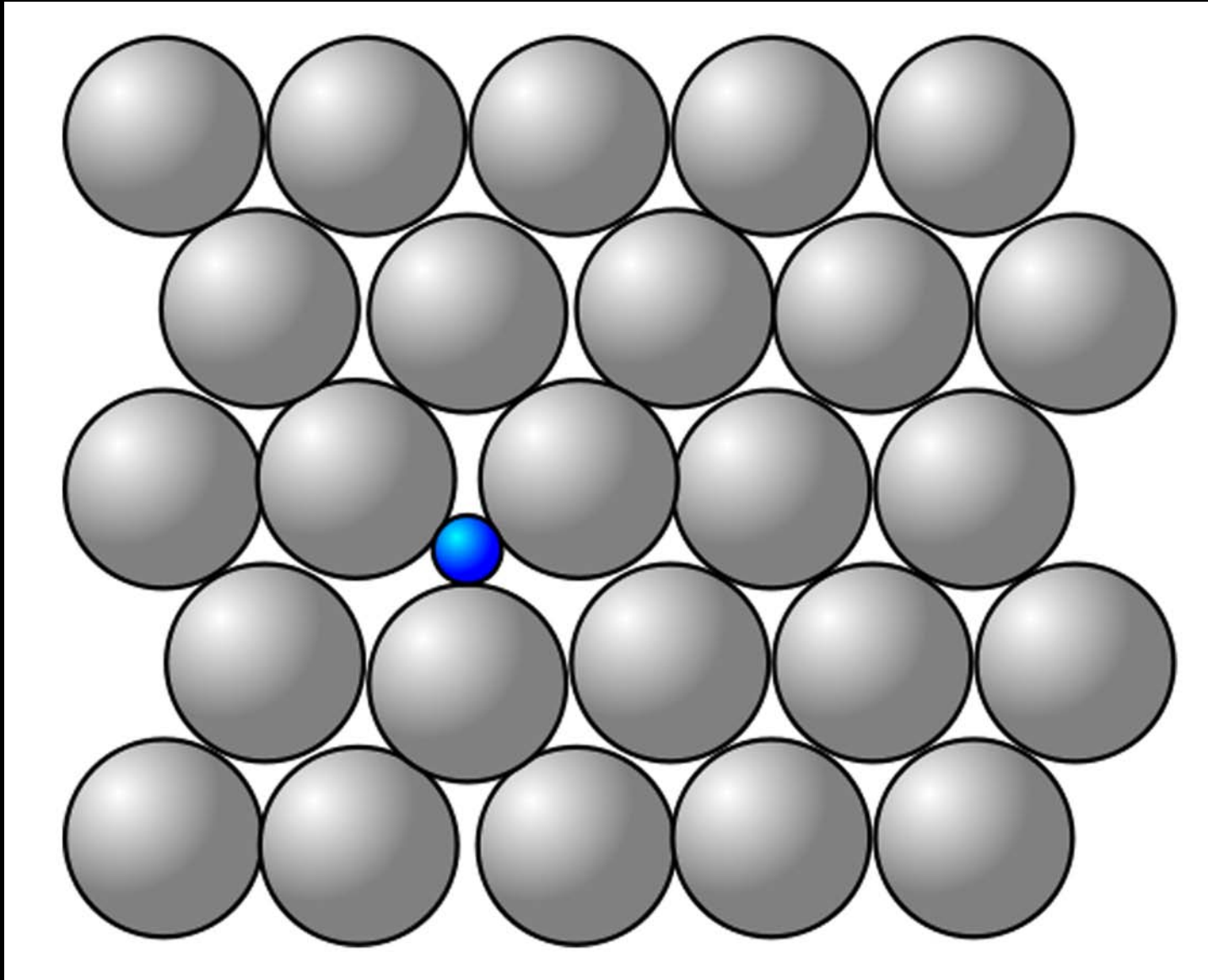


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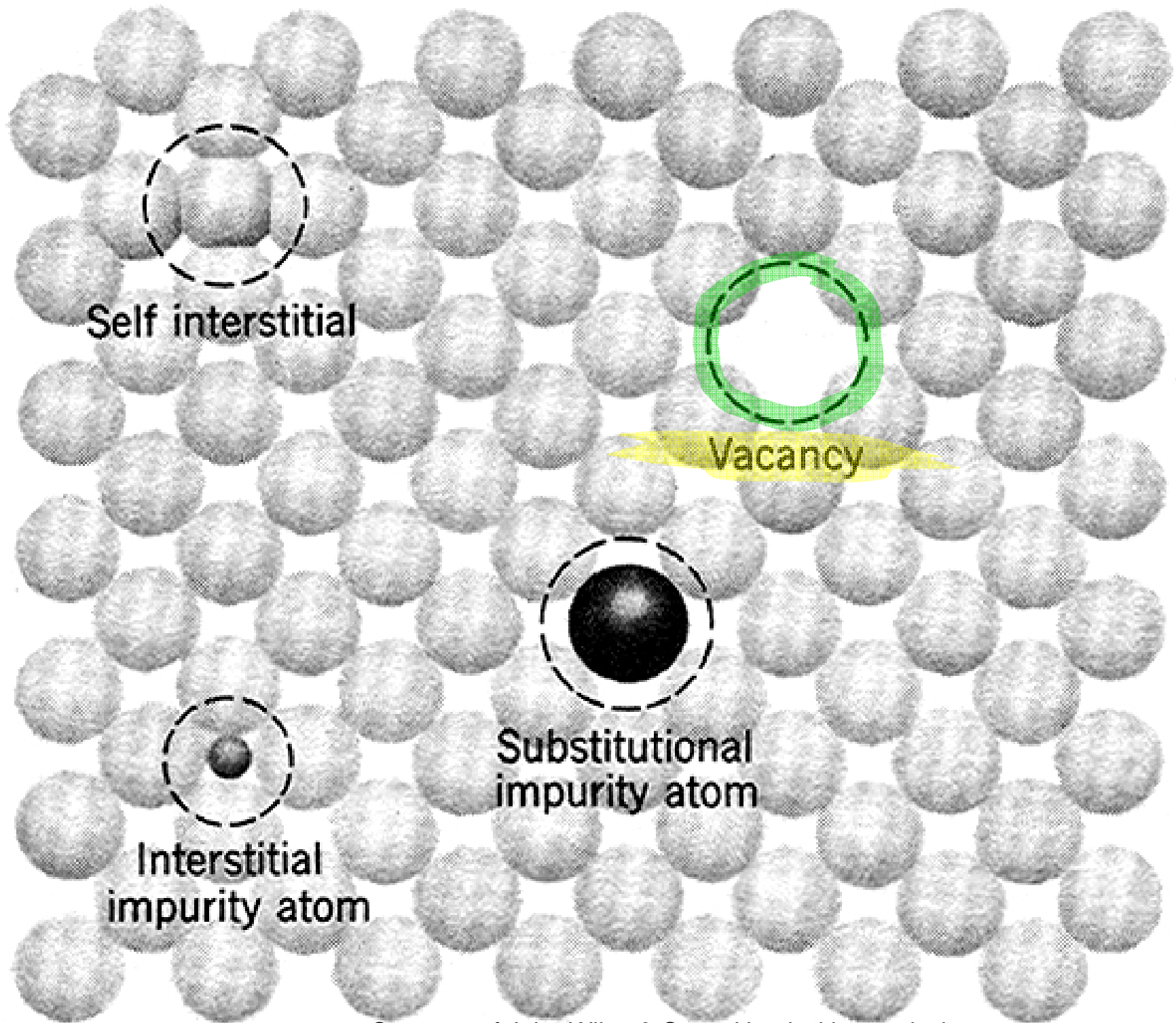
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### **3. Vacancy**

- unoccupied lattice site
- formed at time of crystallization
- formed in service under extreme conditions



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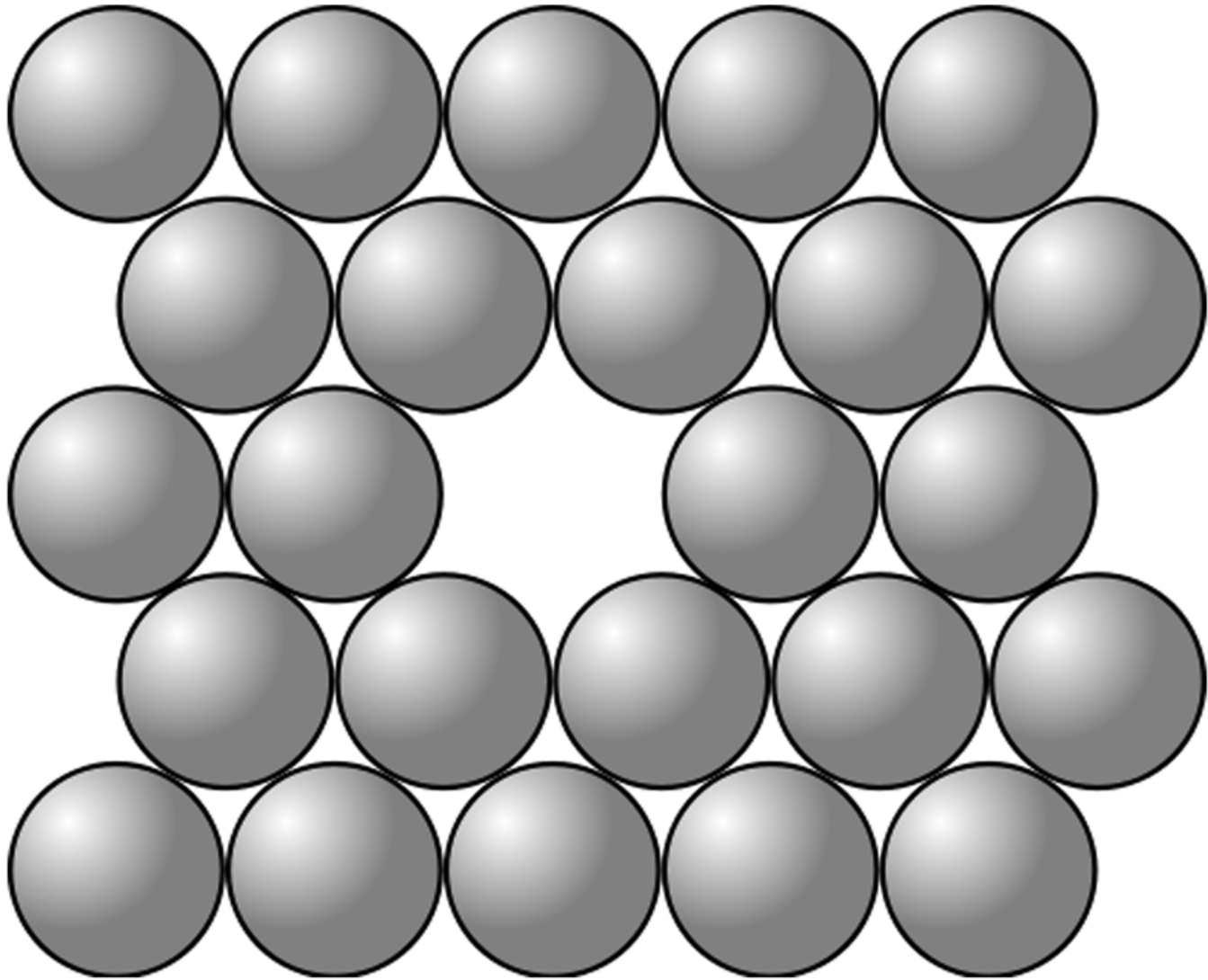


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## Monovacancies and divacancies in copper Reanalysis of experimental data

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### Abstract

The vacancy concentrations  $c_v$  in copper measured by means of the absolute technique (Hehenkamp et al., Phys. Rev. B 45 (1992) 1998) and those derived from positron lifetime studies (Kluin, Philos. Mag A 65 (1992) 1263) are reanalysed. Taking into account the results of quenching and annealing investigations the best fit to the temperature function of  $c_v$  is described by  $H_{1v}^F = 1.03$  eV and  $S_{1v}^F/k = 1.1$  for the monovacancy formation enthalpy and entropy and a divacancy binding enthalpy and entropy of  $H_{2v}^B = -0.23$  eV (attractive interaction) and  $S_{2v}^B/k = 2.8$ , respectively. Accordingly, the divacancy concentration amounts to  $1.5 \times 10^{-4}$  at the melting temperature. © 1999 Elsevier Science B.V. All rights reserved.

*Keywords:* Vacancies; Monovacancies; Divacancies; Copper

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## **Point Defects in Ionic Crystals**

- special issues associated with the need to maintain global charge neutrality

### **1. Schottky Imperfection**

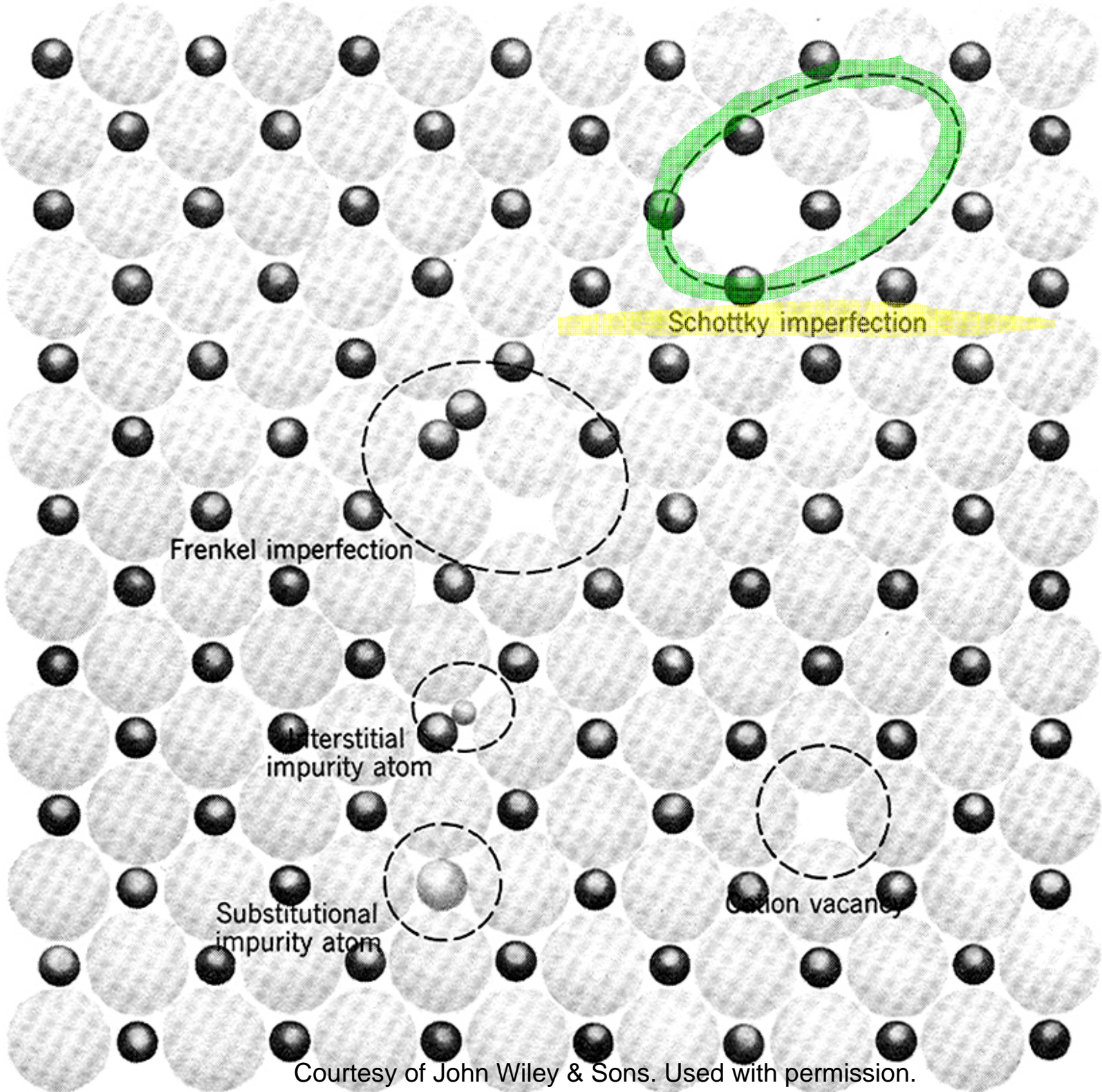
- formation of equivalent (not necessarily equal) numbers of cationic and anionic vacancies

### **2. Frenkel Imperfection**

- formation of an ion vacancy and an ion interstitial

### **3. F-Center**

- formation of an ion vacancy and bound electron



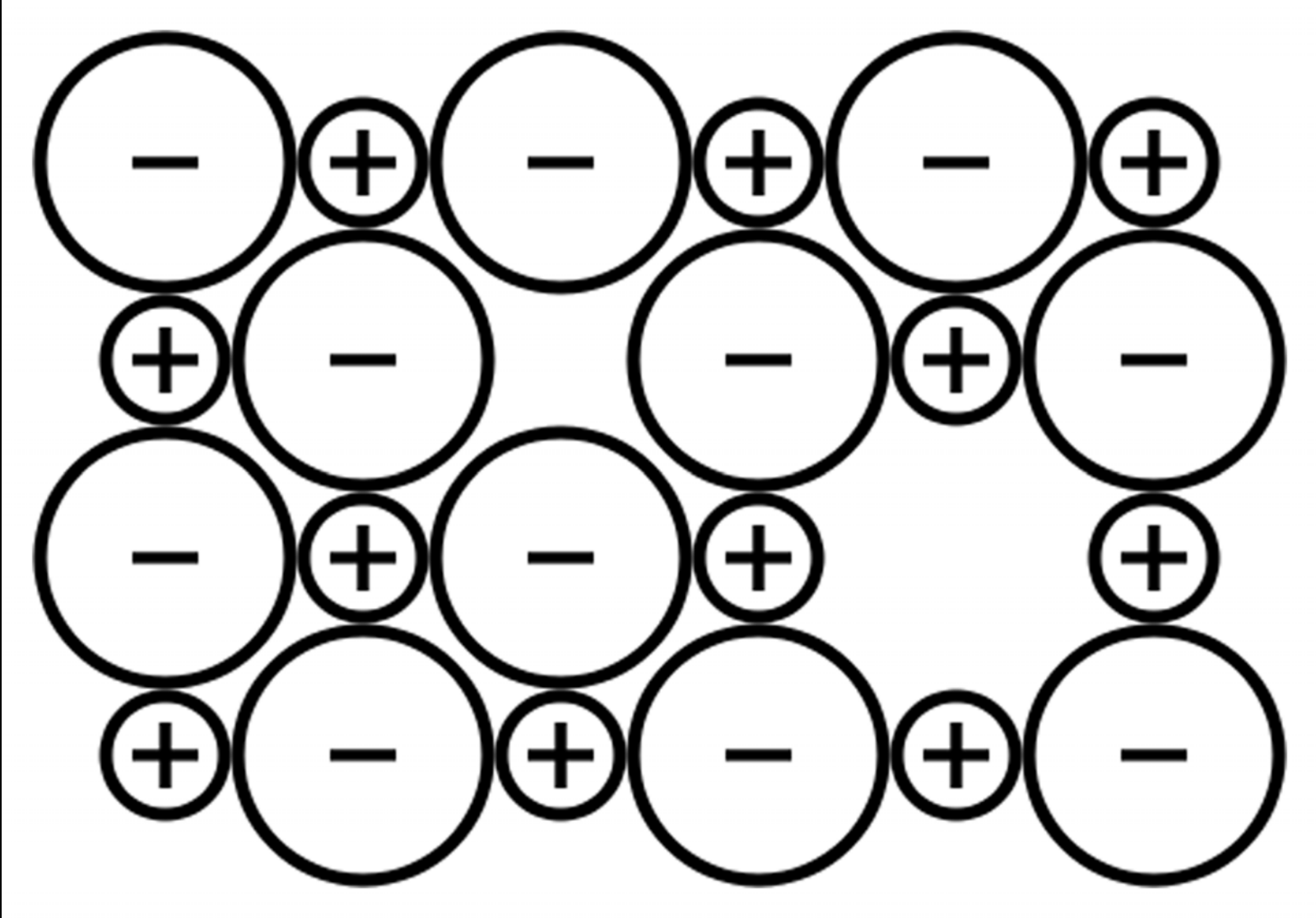


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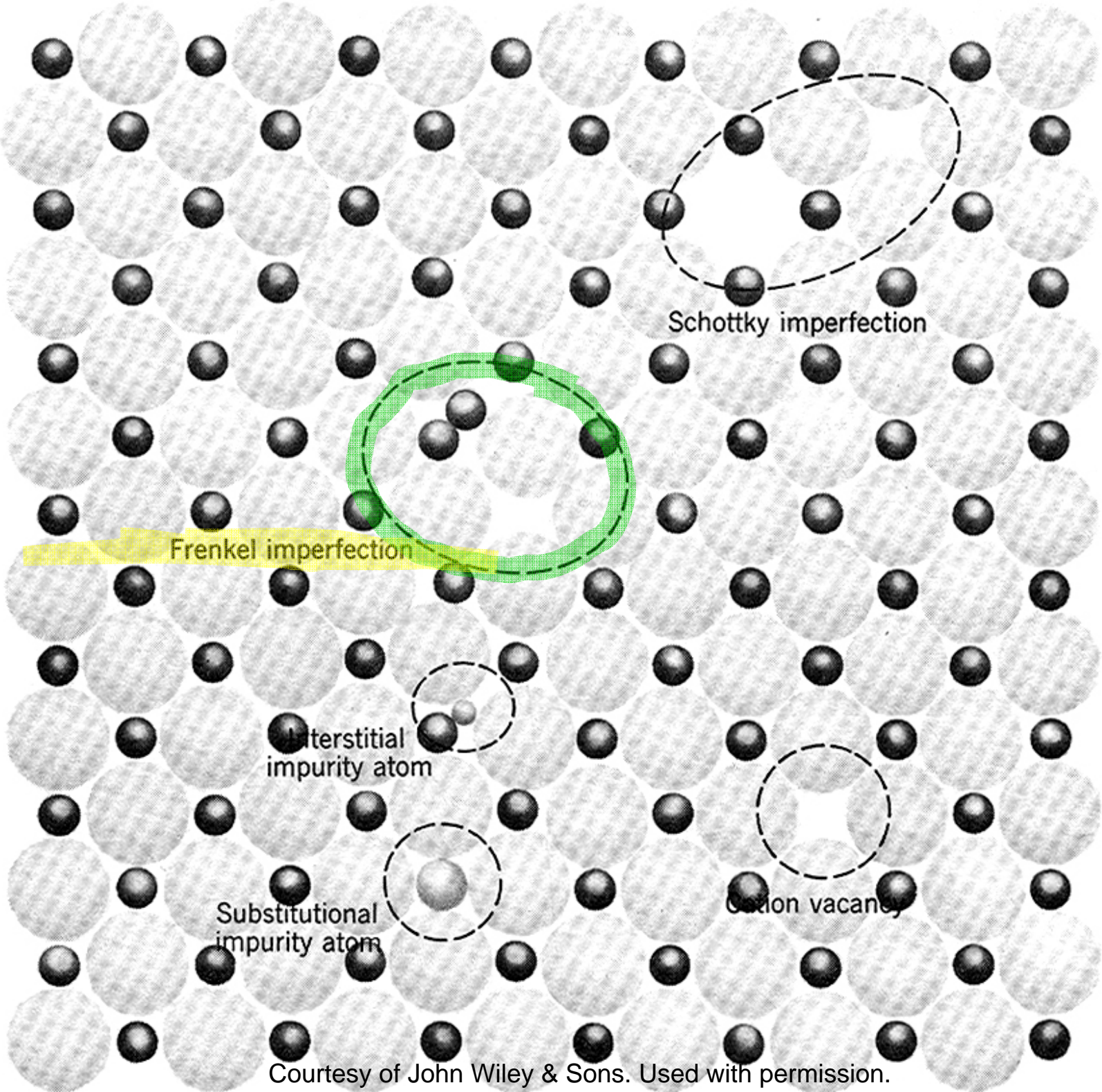
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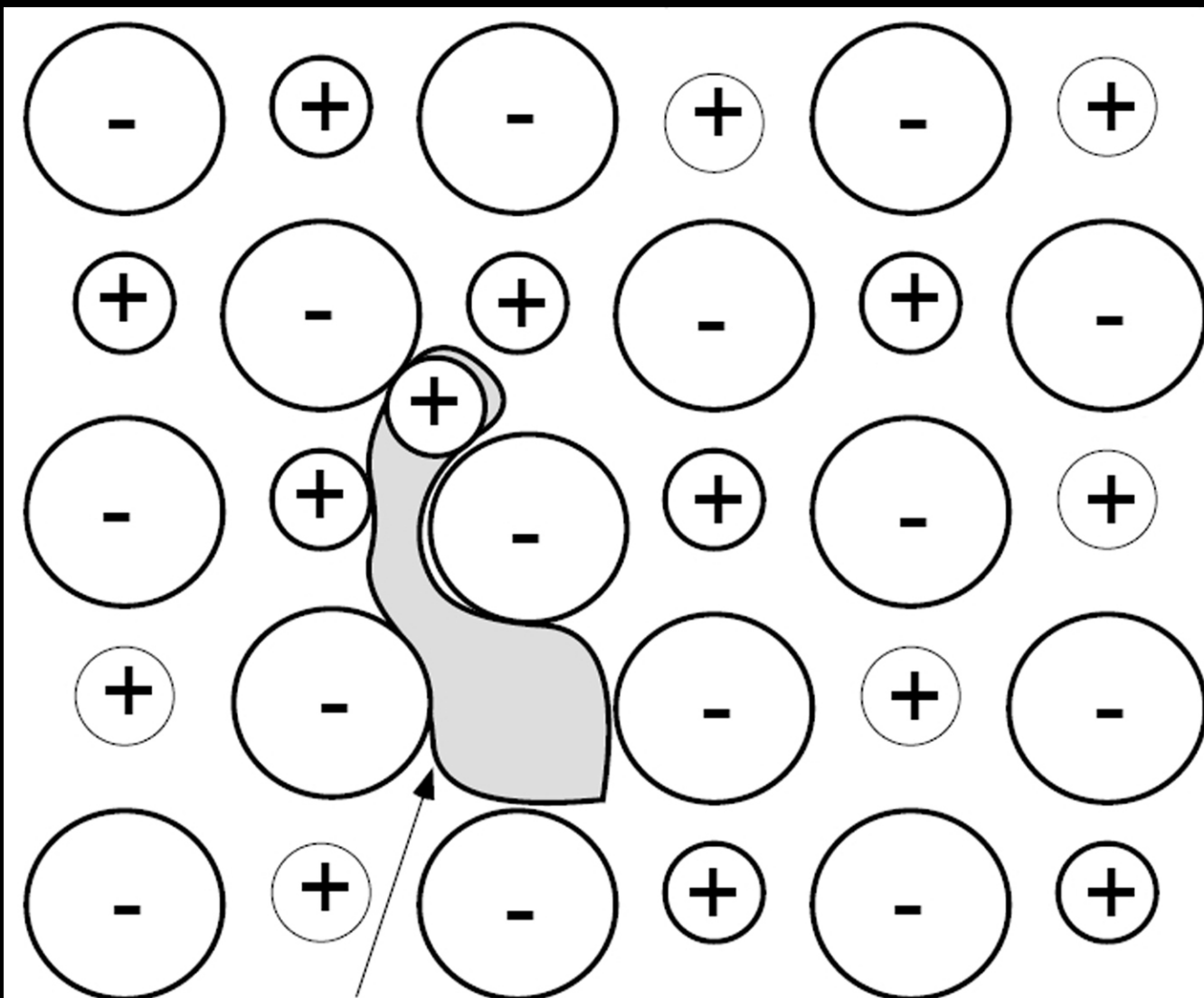
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Frenkel defect

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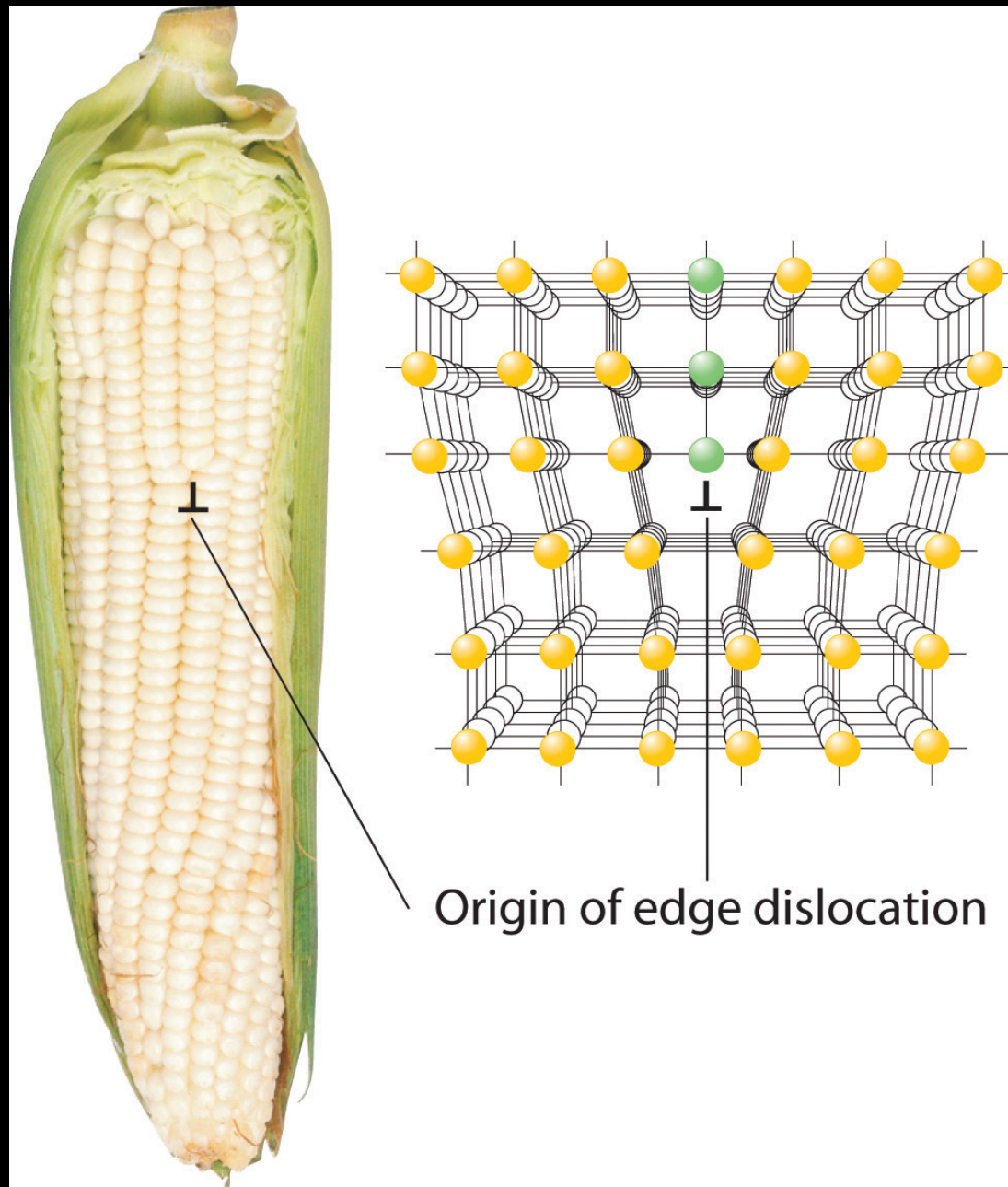
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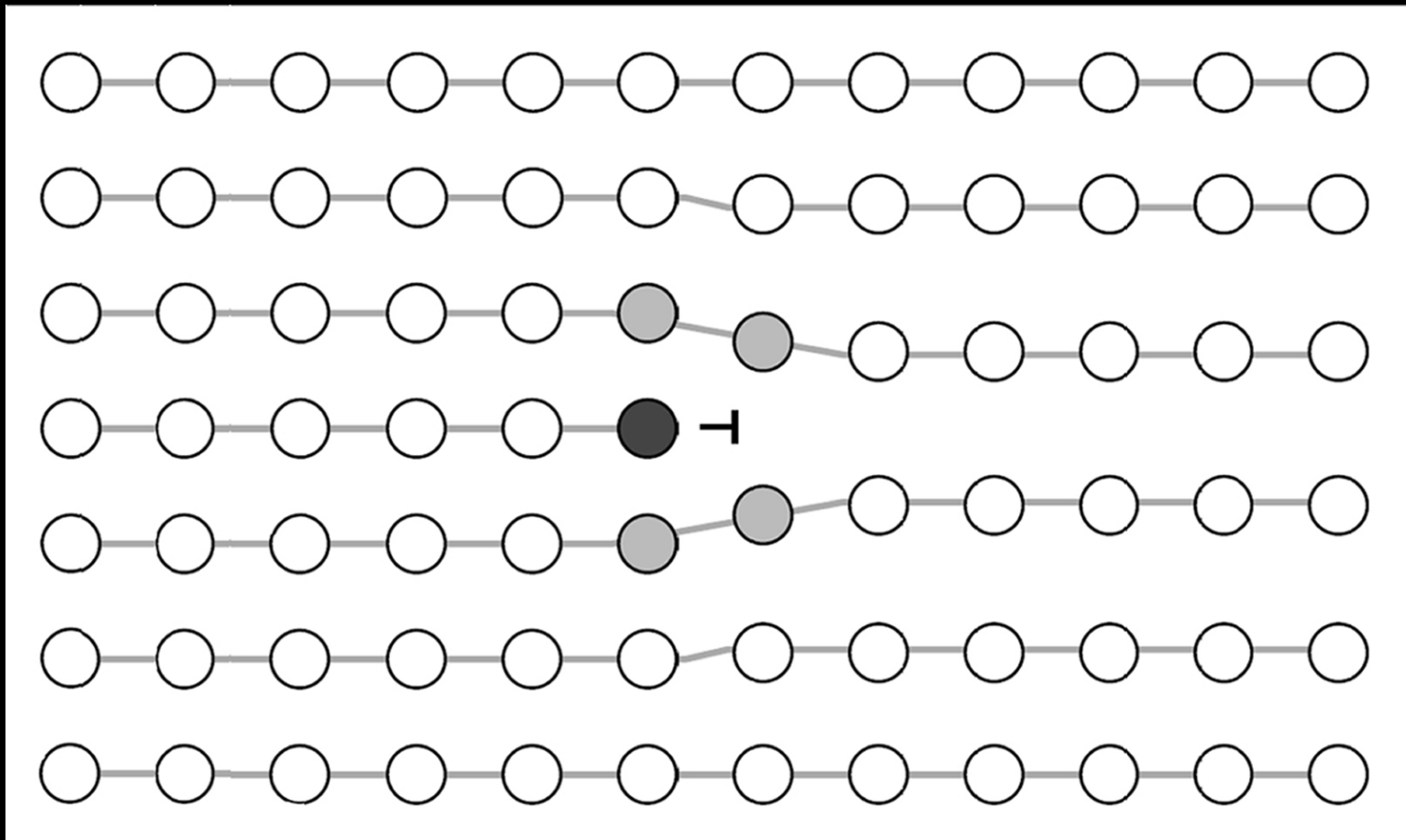
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Averill, B., and P. Eldredge. *Chemistry: Principles, Patterns, and Applications*. Flat World Knowledge, 2011. ISBN: 9781453331224.



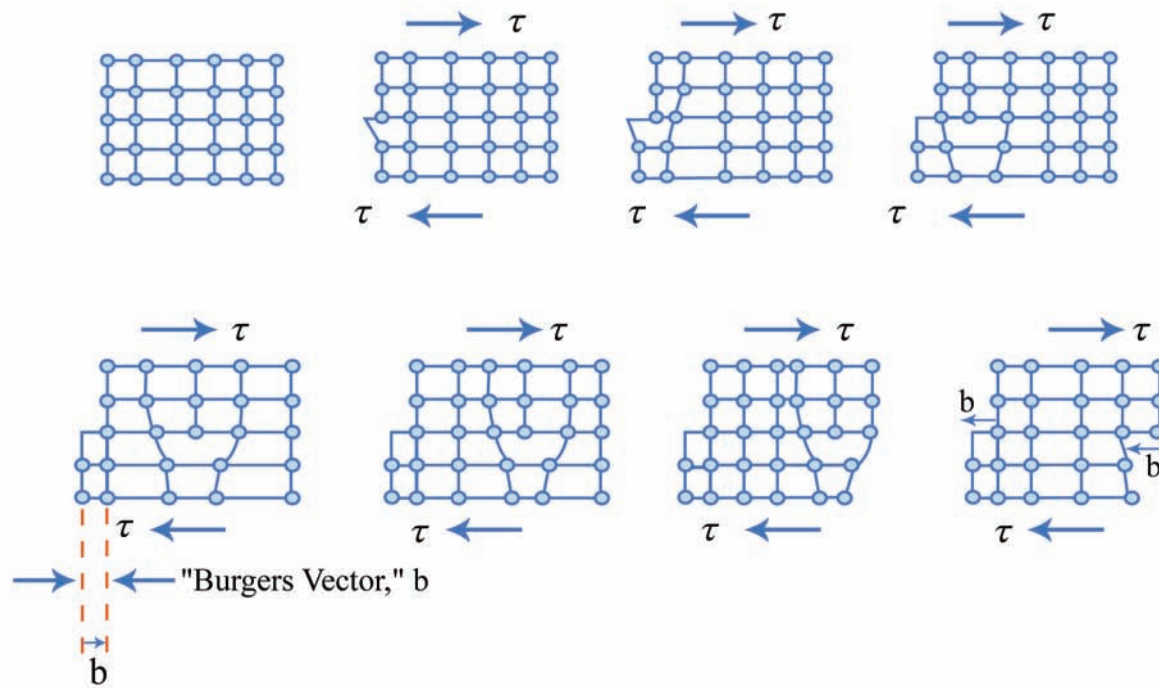


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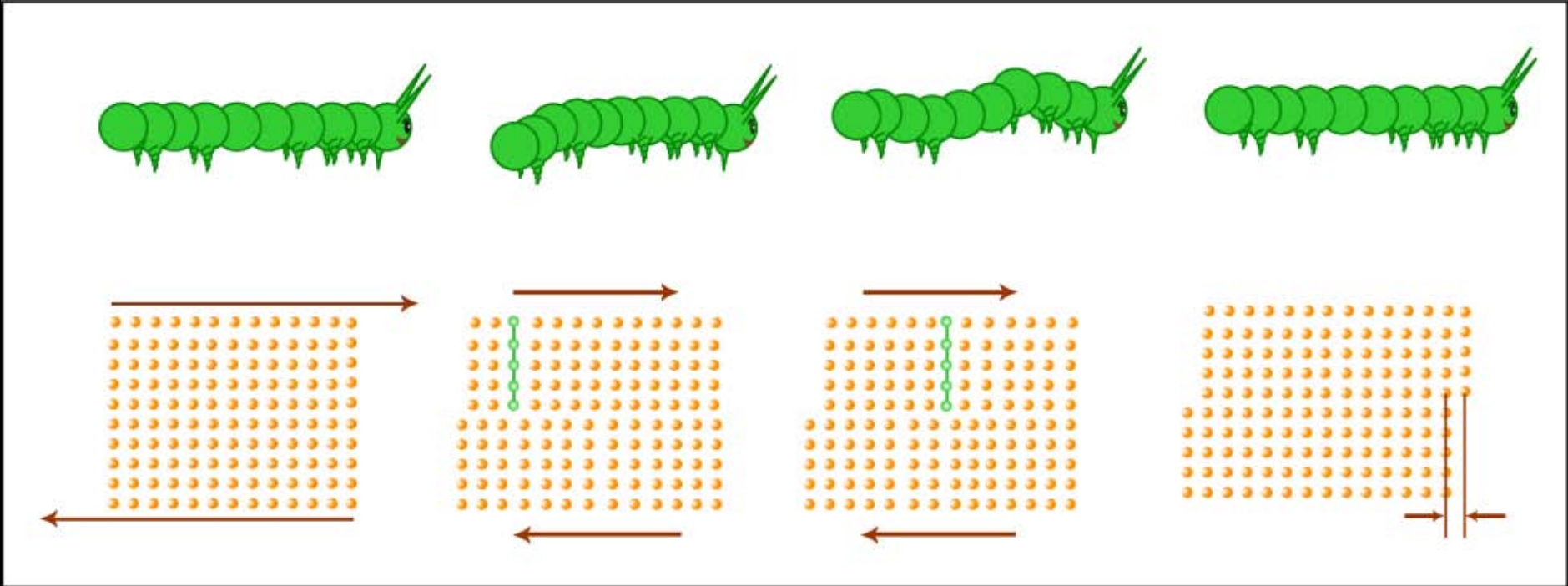
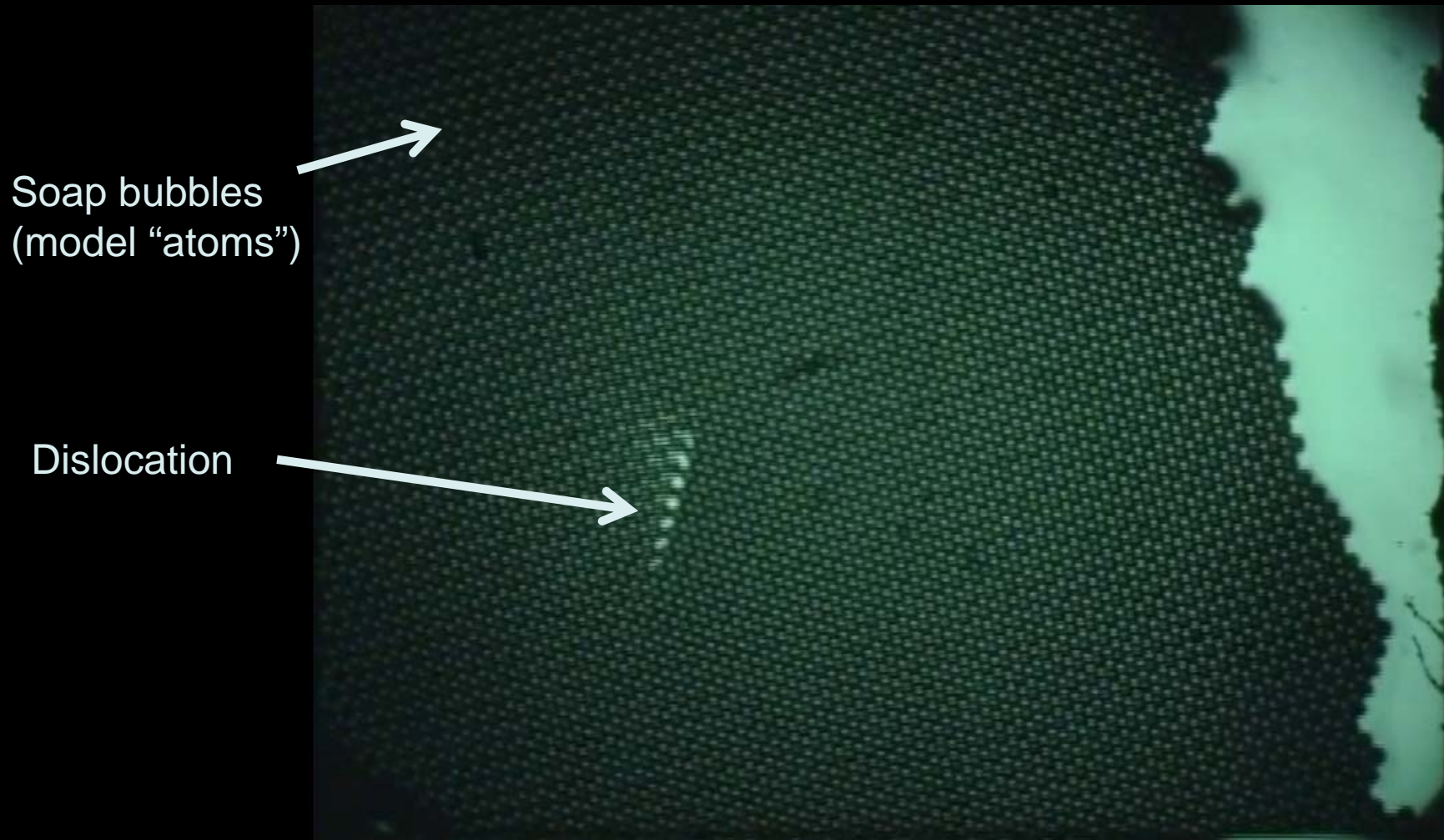


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# Modeling dislocations in a soap bubble raft (Bragg and Nye)



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Fall 2009

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