

**Teaser Question**  
**Basic Training in Condensed-Matter Theory**

James Sethna; Due Friday, January 30, 2009

Last revised: January 27, 2009, 7:55 pm

**Vacancy interactions**

We will show in class that the elastic interaction between vacancies in an elastically isotropic crystal vanishes to dipolar order. (The elastic dipole displacement field for a vacancy at the origin  $\mathbf{u}(\mathbf{r}) = \Delta V \hat{\mathbf{r}} / (4\pi r^2)$  propagates the net volume change  $\Delta V$  to infinity, so there is no compressive stress or strain to couple to the other vacancies.) I may be ignorant, but I don't know the leading order elastic interaction between vacancies – its physical origin, magnitude, or even sign. Once we go beyond isotropic linear elastic theory, there are lots of options for interaction mechanisms.

1. Higher multipoles. What is the second non-vanishing elastic multipole for an on-site vacancy in a cubic crystal? (I'm not sure of a good reference for this, but I did dig up Shuey and Beyeler, <http://www.springerlink.com/content/n527r54278371023/fulltext.pdf>.)
2. Anisotropic elasticity. (What is the strain field around a vacancy in a cubic crystal with  $C_{44}$  not equal to  $(C_{11} - C_{12})/2$ ?)
3. Dispersion. (What are the effects of corrections to the Debye spectrum  $\omega(k) \propto k$ ?)
4. Nonlinear elasticity. What are the effects of corrections to Hooke's law? (Nonlinear elastic terms are usually ignorable because the material fails before they become important. (Apart from rubbers and other exotic materials, most materials either reach their fracture toughness or their yield stress well below 1% strain, where nonlinear terms would normally be around 1% of the linear term.) But near a defect, strains can be very large – there is no room for a crack or a dislocation within one or two atomic lengths of a vacancy or a dislocation.)

To set up notation (in a perhaps non-standard way), use the expansion of the isotropic elastic free energy in powers of gradients of the strain field:

$$\begin{aligned}
 \mathcal{F}(x) = & (1/2)\lambda\varepsilon_{ii}^2 + \mu\varepsilon_{ij}^2 && \text{(linear, isotropic)} \\
 & + C_1^{3,0}\varepsilon_{ij}\varepsilon_{jk}\varepsilon_{ki} + C_2^{3,0}\varepsilon_{ii}\varepsilon_{jk}^2 + C_3^{3,0}\varepsilon_{ii}^3 + \dots && \text{(cubic nonlinear)} \\
 & + C_1^{2,2}(\partial_i\varepsilon_{ij})(\partial_j\varepsilon_{kk}) + \dots + C_{11}^{2,2}\partial_i(\varepsilon_{jk}\partial_i\varepsilon_{jk}) + \dots && \text{(dispersion)} \\
 & + C_1^{4,0}\varepsilon_{ij}\varepsilon_{jk}\varepsilon_{kl}\varepsilon_{li} + \dots + C_5^{4,0}\varepsilon_{ii}^4 + \dots && \text{(quartic nonlinear)}
 \end{aligned}$$

5. Geometric nonlinearity. (The strain tensor  $\varepsilon_{ij}$  is in fact not linear in the displacement fields  $u_i$ ;

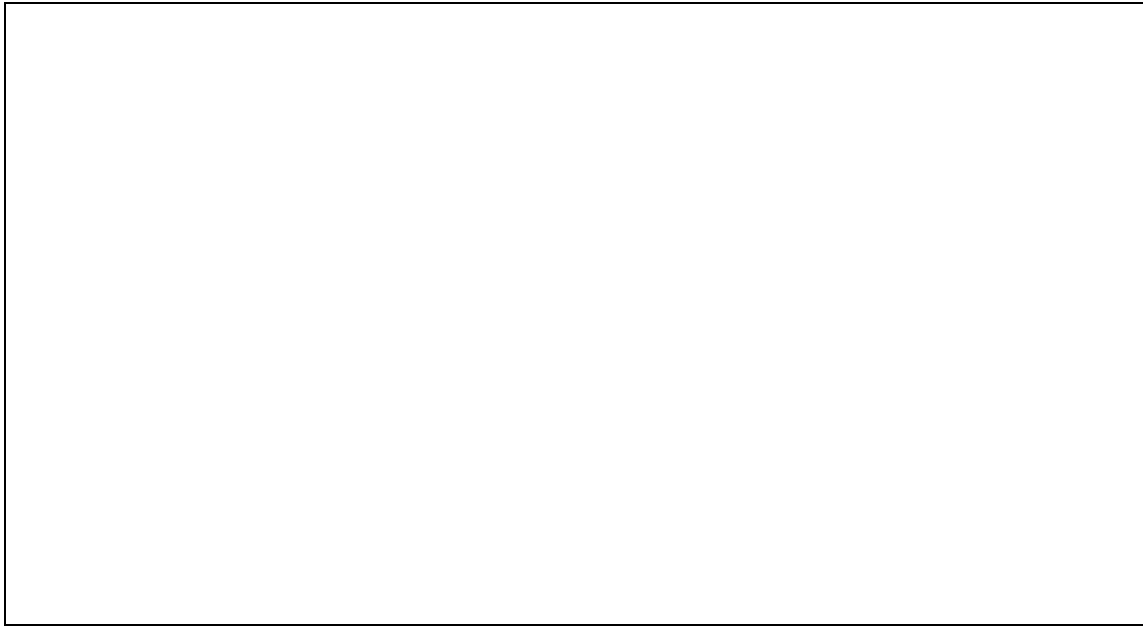
$$\varepsilon_{kl} = \frac{1}{2}(\partial_k u_l + \partial_l u_k \pm \partial_k u_m \partial_l u_m)$$

with the last term depending on whether Eulerian or Lagrangian coordinates are being used (see Chaiken and Lubensky). This geometric nonlinearity is often neglected.

These higher order effects could be relevant for experiments with vacancies. (Will they clump into void? Could a mutual repulsion lead to corrections to the diffusion equation?) Also, one could get much faster convergence for electronic structure calculations if one knew the interactions to high order. Knowing the

leading interaction between vacancies is important if your periodic boundary conditions can only generate periodic arrays. See “Ab initio study of screw dislocations in Mo and Ta: A new picture of plasticity in bcc transition metals”, S. Ismail-Beigi and Tomás A. Arias, *Phys. Rev. Lett.* **84** 1499-1502 (2000) for an example where the leading interactions between the periodic array of dislocations were subtracted off to get the dislocation energy.

*Break up into groups, and each group pick one candidate mechanism. Estimate the leading-order power-law interaction due to your mechanism.*



*Answer in box above. Bring to class Friday.*

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