Is it possible the \textit{ab initio} thermodynamics with defects?

In Gee Kim
Computational Metallurgy Laboratory,
GIFT, POSTECH, Pohang 790-784
Phase-Diagrams: The first-step of materials design

Process design with kinetics


Defects generate heat, e.g., Potevine-LeChatelier (PLC) effect

Chen et al., ISIJ Int. 47, 1804 (2007)

Fig. 1. (a) Stress-strain curve of Fe6.6CuFe TWP steel. (b) Enlargement of the first boxed segment of the stress-strain curve exhibiting type A serrations, characterized by a steep rise in stress alternating with plateau-like features. (c) Enlargement of a typical type A serration. The steep rise corresponds to the initiation of a PLC band outside the strain gauge measuring range. The plateau segment corresponds to the passage of the PLC band in the strain gauge measuring range. The increase in stress in the plateau segment suggests strain hardening in the region outside the PLC band. (d) Enlargement of the type B serrations, characterized by a sawtooth serration pattern.

Fig. 8. (a) Low SFE model: a low SFE leads to widely dissociated partial dislocations, which cannot cross slip. This pronounced planar slip results in a high strain hardening rate. (b) Dynamic Hall–Petch model of Bouaziz–Guelton: at low SFE, twinning is promoted. The intersection of twins forms a cell structure. The twin boundaries act as obstacles for dislocation glide. (c) Planar slip model: in concentrated solid solution alloys short range order (SRO) is possible and dislocations will destroy the SRO on their slip plane. Whereas the leading dislocation experiences a high resistance to its motion, subsequent dislocations can glide more easily in the same slip plane. This favors planar slip and result in a high rate of strain hardening. (d) Illustration of the reduction of the SRO during the passage of partial dislocation on their glide plane: the octahedral clusters are sheared and the C atoms are transferred to tetrahedral interstitial sites. Left: before slip. Right: after slip. (e) Dastur–Leslie model: dynamic strain aging in FeMnC alloy is caused by the re-orientation of Mn–C cluster in the dislocation stress field during dislocation motion.
A material as a system by multiscale simulation

Courtesy by G. B. Olson, Dept. MSE, Northwestern Univ., USA
Technology Transfer

Questek® Navy Alloy Designs

EFV—Cast Stainless Suspension Components

JSF—Be-free High Strength Cuprium™

Seahawk—Prognosis Smart Steel

CVN21—CS130 Deck Steel

Naval EM Railgun—Armature Alloy

LHA-6—AA5xxx Accelerated Qualification

ONR: N00014-05-M-0250
NAVIAIR: N68335-06-C-0339

ONR: N00014-07-M-0445 STTR-I

Seahawk

SCC-Resistant Structural Al

Considering the images and text, the following projects are highlighted:

- **EFV**: Cast Stainless Suspension Components
- **JSF**: Be-free High Strength Cuprium™
- **Seahawk**: Prognosis Smart Steel
- **CVN21**: CS130 Deck Steel
- **Naval EM Railgun**: Armature Alloy
- **LHA-6**: AA5xxx Accelerated Qualification

The associated projects and contracts include:

- **ONR**: N00014-05-M-0250, N00014-07-M-0445 STTR-I
- **NAVIAIR**: N68335-06-C-0339, N68335-07-C-0428
- **NAVIAIR**: N68335-05-C-0207, N68335-07-C-0108

These projects are part of various military programs, including F/A-18E/F Super Hornet, CVN-21, JSF, and others, demonstrating advancements in material science and technology transfer.
“I do not accept that this is a philosophical difficulty, or that it demonstrates anything like an impossibility *in principle* of treating macroscopic objects quantum-mechanically; merely that this discussion brings out the *practical* problems of determining all the relevant phases in a given system.”

Geometric theory of defects

Elastic deformation (Euclidean)

Riemann-Cartan manifold theory

Levi-Civita connection (Christoffel symbols)

Curvature tensor of the affine connection

torsion

nonmetricity

The ground undeformed state of the medium ➔ The external observer fixes a Cartesian coordinate system (Gauge fixing).

The deformed medium, ➔ The external observer discovers that the metric becomes nontrivial in this coordinate system.

Topological defects ➔ Einstein equation for 3D gravity

Katanaev, Phys. Usp. 48, 675 (2005)
Example: Dislocations

Burgers vectors constructed by the Volterra process

- **Invariant** under arbitrary coordinate transformation,
- **Covariant** under global SO(3) rotations of \( y^i \).

With the Cartan torsion tensor \( T \)
Single-particle quantum motion on a Riemann-Cartan manifold

The tight-binding Hamiltonian

The distortions by defects

The affine connection and the covariant derivative

with the torsion tensor, measures the defect density.

The new Hamiltonian with defects for the continuum limit $a \to 0$
Aharonov-Bohm effect of the spin wave by a screw dislocation

We shall now present the solution of equation (10) for a single screw dislocation along the \( z \) axis with the Burgers vector \( b = b e_z \). The only nonvanishing components of the Kröner distortions \( \beta_j^i \) are then \( \beta_1^3, \beta_2^3 \):}

\[
\beta_1^3 = -\frac{b}{2\pi} \partial_2 \ln \sqrt{(x^1)^2 + (x^2)^2},
\]

\[
\beta_2^3 = \frac{b}{2\pi} \partial_1 \ln \sqrt{(x^1)^2 + (x^2)^2}.
\]

Assuming in the cylindrical coordinates \( \Psi(r, \phi, z, t) = \chi(r, \phi) \exp(ikz + i\omega t) \) we found that the envelope \( \chi(r, \phi) \) obeys the Aharonov–Bohm equation [18]:

\[
\left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left( \frac{\partial}{\partial \phi} + i\alpha \right)^2 - q^2 \right] \chi(r, \phi) = 0,
\]

where \( \alpha = kb/2\pi \) and \( q^2 = k^2 + 2\mu \omega \). Using the asymptotic \( r \rightarrow \infty \) solution for that equation [12, 18–20] and recalling the definition of the function \( \Psi \) we found

\[
\begin{pmatrix}
\delta S_x \\
\delta S_y
\end{pmatrix} = S_0 \begin{pmatrix}
\cos \pi \alpha \\
-\sin \pi \alpha
\end{pmatrix} (q r + \alpha (\phi - \pi)/2|\alpha| - \pi/4).
\]

(13)

In the absence of the dislocation the (pseudo)flux \( \alpha = 0 \) and we recover the standard spin wave solution of equation (1). The first term on the rhs of equation (13) shows the helical structure of the incoming spin wave due to global distortion of the lattice and the second describes the scattering phase shift due to the presence of dislocation. In figure 1 we have shown a Mathematica 7 generated density plot for the \( \delta S_y \) component of the solution (13). The \( \delta S_x \) component exhibits an identical structure with a trivial phase shift found from (13).

Figure 1. Mathematica 7 density plot for spin wave \( S_y \) solution equation (13). The wave is approaching from the right and deflects from the screw dislocation line located at the origin and perpendicular to the plot surface. The wavy edges of the cut to the left from the dislocations show the Aharonov–Bohm-like oscillations determined by the (pseudo)flux \( \alpha = 0.4 \).
Gauge theory of moving dislocations

The dislocation density tensor and the dislocation current tensor

Satisfy the translational Bianchi identities,

The Lagrangian density

The equations of motion

By adding null Lagrangian, satisfying

momentum balance of dislocations
stress balance of dislocations
force balance of elasticity

Usual solution: massive fields Klein-Gordon equation

With (1+2)-dimensional d’Alembert operator,
Matsubara-Green-Kubo formalism

Grand canonical partition function, with

Statistical density matrix, follows the Bloch equation

By introducing the imaginary-time, the temperature Green’s function satisfies the Schwinger-Dyson equation as

with the noninteracting Green’s function

In terms of the spectral function, the Lehmann representation of the Green’s function is

The corresponding real time Green’s function is
Thermodynamics of black holes

Hartle-Hawking-Gibbons-Perry formalism

An action functional

The amplitude

The propagator

Introducing the negative imaginary parametric time

then

satisfies where

\[ S: \text{the square of the Minkowski interval} \]

For the metric,

with the Klein-Gordon Lagrangian density

the diffusion equation,

of the normal mode \( \psi \) yields the partition function

for small \( \beta \).


Conclusion

- A fully quantum field theoretic formalism is available for thermodynamics with defects.
- This approach promises the authentic *ab initio thermodynamics* by eliminating *ad hoc* ones.
- Computational Practicality? See, below simulations by serious scientists.


Two colliding galaxies. By S. Kazantzidis, University of Chicago