A mystery of dissipative motion of radiation defects and dislocations.

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Dissipative motion of defects and dislocations

Über den Einfluß thermisch angeregter Schallwellen auf die plastische Deformation*.

Von

GÜNTHER LEIBFRIED.

Zeitschrift für Physik, Bd. 127, S. 344--356 (1950).

Influence of the thermally excited sound waves on the plastic deformation.

The interaction of kinks and elastic waves

BY J. D. ESHELBY
Department of Physical Metallurgy, University of Birmingham

(Communicated by G. V. Raynor, F.R.S.—Received 3 August 1961)

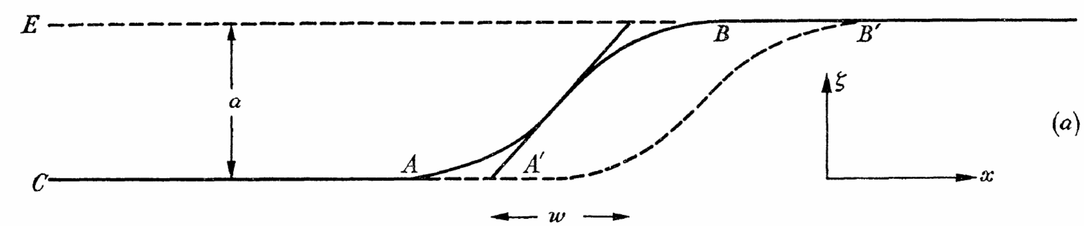
Proc. R. Soc. Lond. A 1962 **266**

Dissipative motion of defects and dislocations

Leibried (1950) finds that a dislocation propagating through a crystal, experiences drag force due to acoustic phonons, where the magnitude of the force per unit length is proportional to temperature

$$\bar{K} = -\sigma \frac{v}{c_t} \cdot \frac{\bar{\varepsilon}}{10}. \qquad \bar{\varepsilon} = \frac{3kTz}{\lambda^3}$$

Eshelby (1962) developed this argument further and applied it to kinks on dislocation lines.



It is easy to show that unless the kink is supersonic (a possibility we do not consider) (6·5) is incompatible with the equation of energy conservation

$$\hbar^2 K^2/2m = \hbar^2 K'^2/2m \pm \hbar c k,$$

and so we must consider second-order transitions.

Dissipative motion of defects and dislocations

Argument involving the incompatibility of the dispersion relations of quasiparticles with different dispersion relations is well known. Absorption or emission of a single phonon by a massive (i.e. *not* mass-less, like a phonon) particle requires that

$$\mathbf{p}' = \mathbf{p} + \hbar\mathbf{k}$$

$$\frac{\mathbf{p}'^2}{2m} = \frac{\mathbf{p}^2}{2m} + \hbar c\,|\mathbf{k}|$$

From the second of the above equations we find that

$$\frac{(\mathbf{p}'-\mathbf{p})\cdot(\mathbf{p}'+\mathbf{p})}{2m} = \frac{\hbar\mathbf{k}\cdot(\mathbf{p}'+\mathbf{p})}{2m} = \hbar c\,|\mathbf{k}|$$

- The latter equation cannot possibly be satisfied unless *(p/m)* is close to the speed of sound, which is never the case under reasonable, i.e. not “the end of the world”, deformation strain rate conditions.
- Hence the occurence of thermal dislocation drag, and in fact any thermal friction experienced by a massive defect, must be fundamentally related to the two-phonon scattering processes.

Dissipative motion of defects and dislocations

In a two-phonon process involving the absorption and emission of phonons, the cross-section of momentum transfer is proportional to

$$\overline{\sigma(\mathbf{p}', n_{\mathbf{k}} - 1, n_{\mathbf{k}'} + 1; \mathbf{p}, n_{\mathbf{k}}, n_{\mathbf{k}'})} \sim \bar{n}_{\mathbf{k}}(\bar{n}_{\mathbf{k}'} + 1) - \bar{n}_{\mathbf{k}'}(\bar{n}_{\mathbf{k}} + 1) = \bar{n}_{\mathbf{k}} - \bar{n}_{\mathbf{k}'} \sim \frac{d\bar{n}_{\mathbf{k}}}{dk}$$

The equilibrium phonon occupation numbers are

$$\bar{n}_{\mathbf{k}} = \frac{1}{\exp(\hbar\omega_{\mathbf{k}} / k_B T) - 1} = \frac{k_B T}{\hbar\omega_{\mathbf{k}}} - \frac{1}{2} + O\left(\frac{\hbar\omega_{\mathbf{k}}}{k_B T}\right)$$

In the classical high temperature limit, accessible to conventional molecular dynamics, dislocation drag is predicted to be a linear function of temperature.

Dissipative motion of defects and dislocations

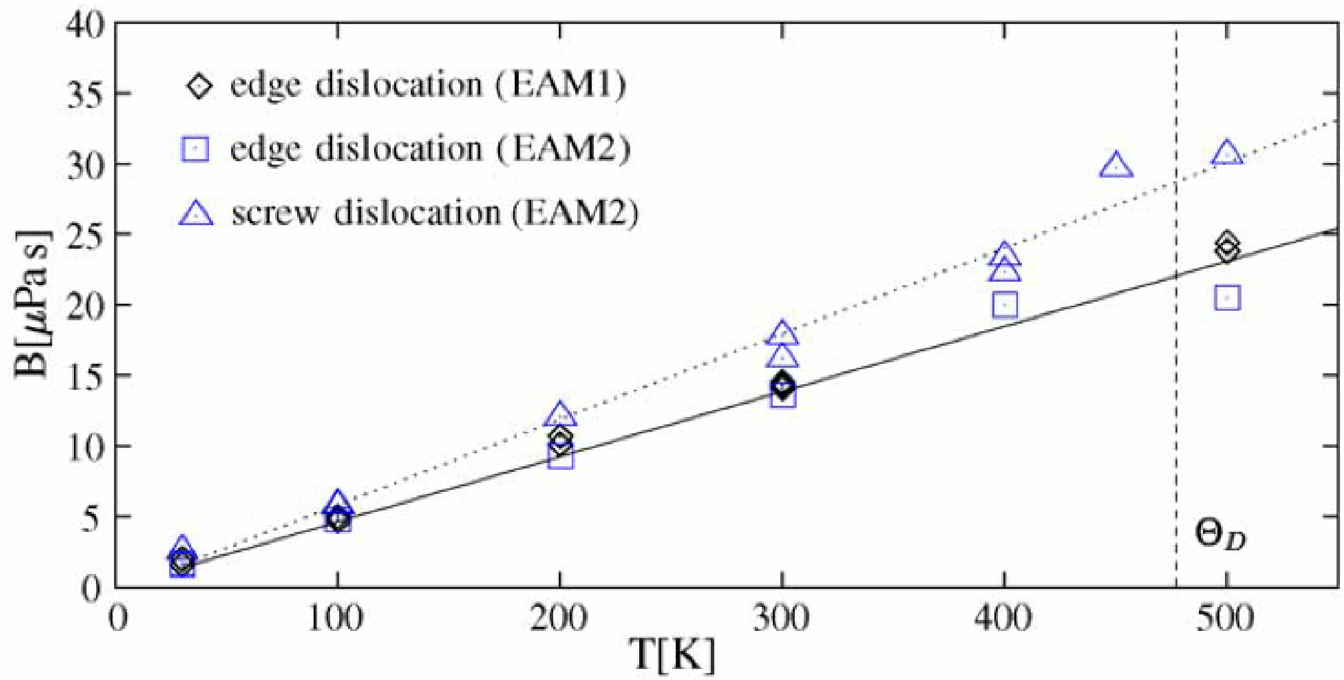
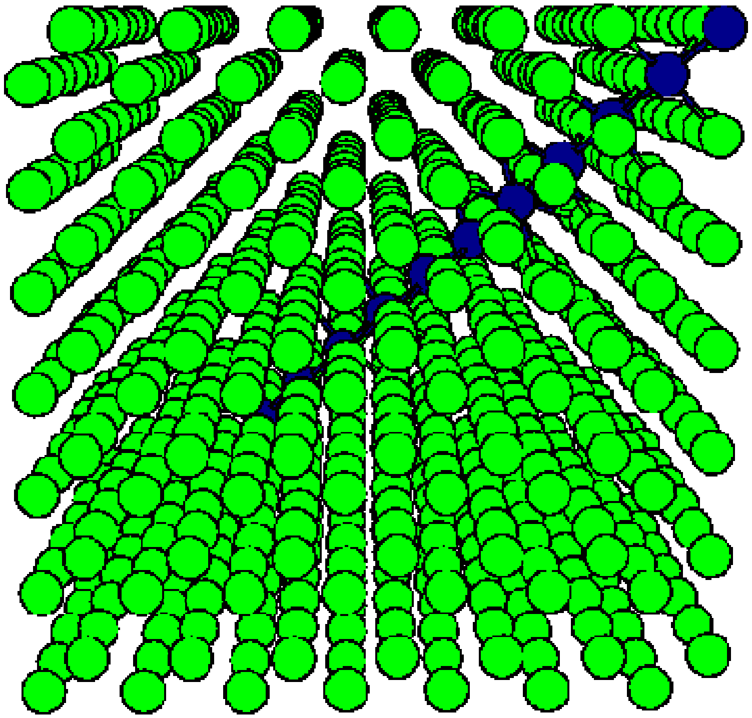


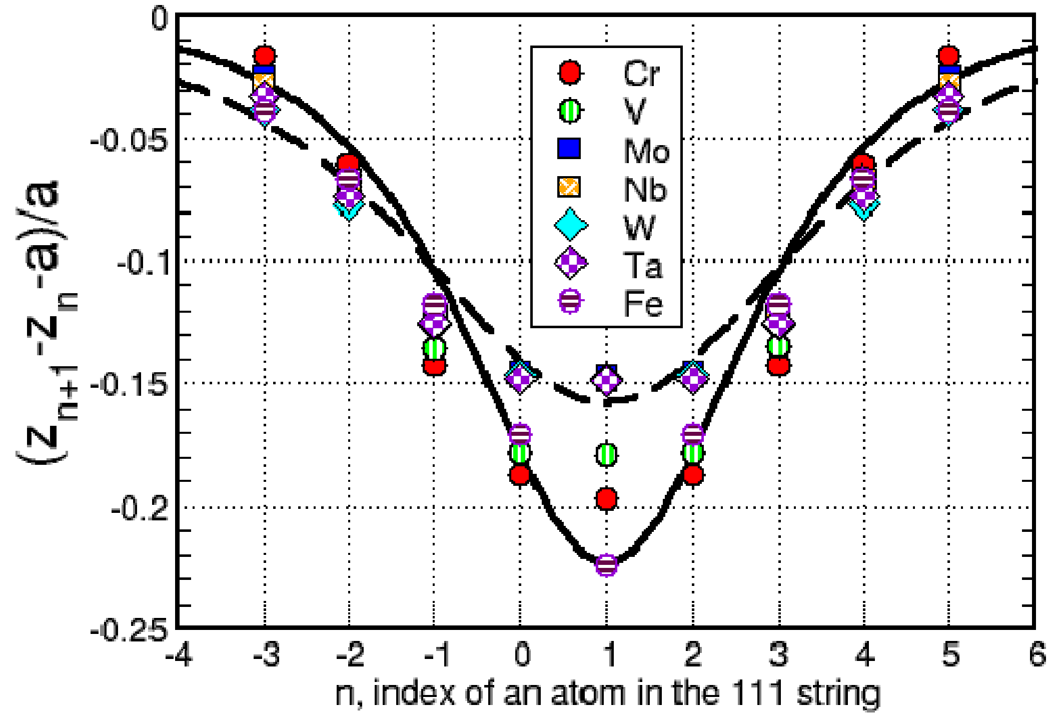
Fig. 1. Drag coefficent for edge and screw dislocations in Ni (blue, EAM1; black, EAM2). The solid line corresponds the Leibfried estimate Eq. (3), Θ_D denotes the Debye temperature.

E. Bitzek, P. Gumbsch, Mater. Sci. Eng. A400/401 (2005) 40

Simulations agree with the Leibfried argument.

Self-interstitial atom defects as massive quasiparticles





$$L=\sum_{n=-\infty}^{\infty}\frac{m\dot{z}^2}{2}-\frac{\alpha}{2}\sum_{n=-\infty}^{\infty}(z_{n+1}-z_n-a)^2-\frac{m\omega_0^2a^2}{2\pi^2}\sum_{n=-\infty}^{\infty}\sin^2\left(\frac{\pi z_n}{a}\right)$$

A crowdion defect is well described by the Frenkel-Kontorova model.

D. Nguyen Manh *et al*. PRB 73, 020101 (2006)

Self-interstitial atom defects as massive quasiparticles

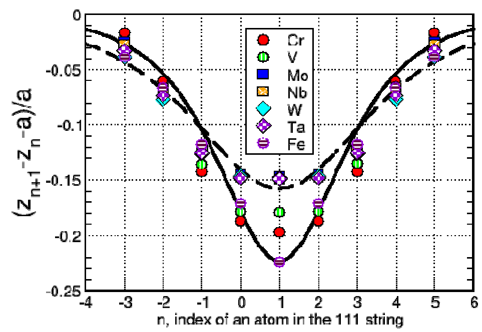
Equations of motion of atoms

$$m\frac{d^2 z}{dt^2} = \alpha(z_{n+1} - z_{n-1} - 2z_n) - \frac{m\omega_0^2 a^2}{2\pi}\sin\left(\frac{2\pi z_n}{a}\right)$$

If the chain of atoms contains an extra atom, the positions of atoms in a chain are described by the following solution

$$z_n(t) = an + \frac{2a}{\pi}\arctan\left[\exp\left(-\frac{\omega_0}{c\sqrt{1 - V^2/c^2}}(an - Vt)\right)\right]$$

The energy of this solution equals



$$E = \frac{Mc^2}{\sqrt{1 - V^2/c^2}} \approx Mc^2 + \frac{MV^2}{2} + \dots$$

Here M is the effective mass of the defect.

The Eshelby-Leibfried treatment is expected to apply.

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Langevin treatment of thermal drag

$$m^* \frac{dv}{dt} = -\gamma v + f(t); \quad f(t) \text{ is the stochastic thermal force.}$$

$$\langle f(t) f(t') \rangle_T = f_T^2 \delta(t-t');$$

$$v(t) = \frac{1}{m^*} \int_{-\infty}^{t} f(\tau) \exp\left(-\frac{\gamma}{m^*}(t-\tau) \right) d\tau$$

FDT: $$m^* \langle v^2(t) \rangle_T / 2 = k_B T / 2 \quad \Rightarrow \quad f_T^2 = 2\gamma k_B T$$

FDT: fluctuation-dissipation theorem

The Langevin equation is consistent with the equipartition principle.

Asymptotic equilibrium FDT condition on the thermal energy of the diffusion particle does not depend on the friction coefficient γ.

Langevin treatment of thermal drag

FDT also makes it possible to establish a relation between the friction coefficient γ and the diffusion coefficient D.

$$v(t) = \frac{1}{m^*} \int_{-\infty}^{t} f(\tau) \exp\left(-\frac{\gamma}{m^*}(t-\tau) \right) d\tau$$

$$\langle v(t) v(t') \rangle_T = \frac{k_B T}{m^*} \exp\left[-\frac{\gamma}{m^*} |t - t'| \right]$$

Position of the defect = integral of its (fluctuating) velocity:

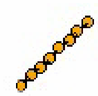
$$x(t) = \int_{-\infty}^{t} d\tau v(\tau); \quad \langle x(t) \rangle_T = 0$$

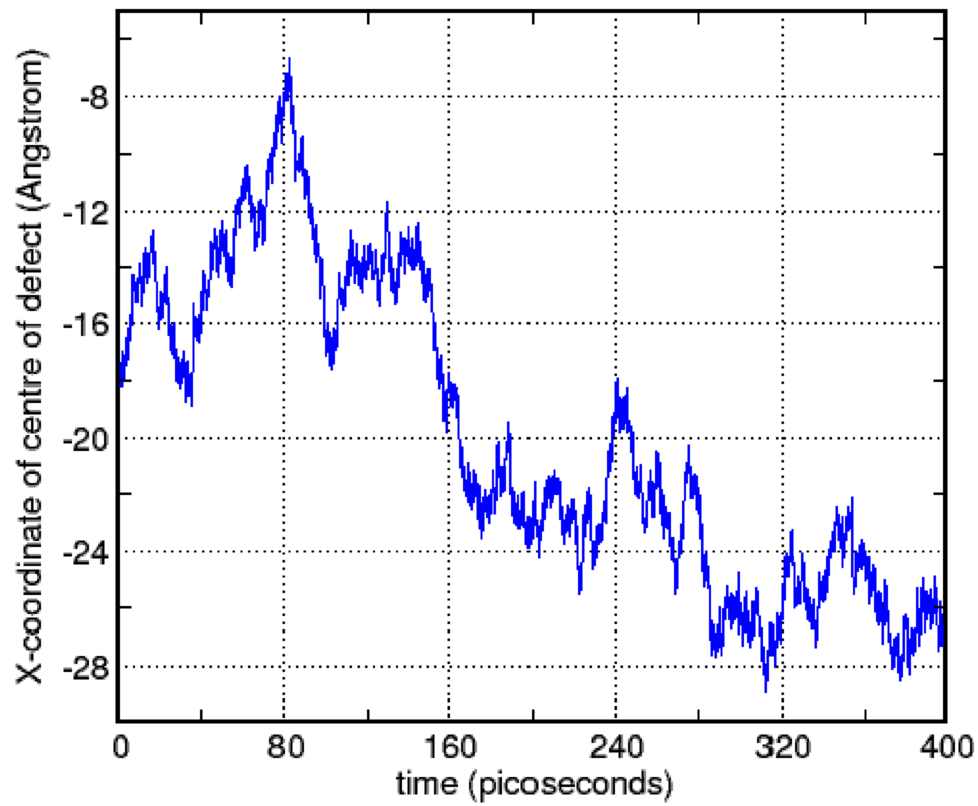
$$\langle x^2(t) \rangle_T = \int_{-\infty}^{t} d\tau \int_{-\infty}^{t} d\tau' \langle v(\tau) v(\tau') \rangle_T$$

$$D(T) = \lim_{t \to \infty} \left[\langle x^2(t) \rangle / 2t \right] = \frac{k_B T}{\gamma(T)}$$

Effective mass m* of the defect is of no significance.

Langevin treatment of thermal drag





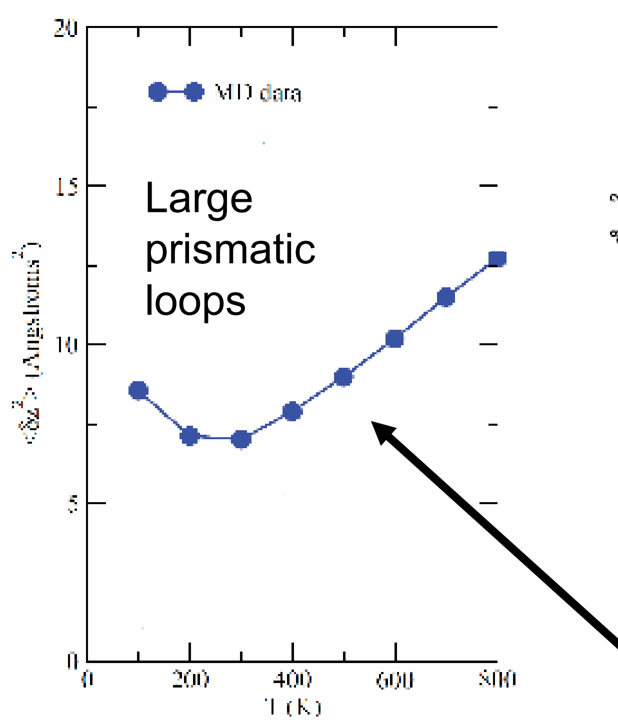
It is possible to extract the values of diffusion coefficient, treated as a function of temperature, directly from the simulated trajectories of defects.

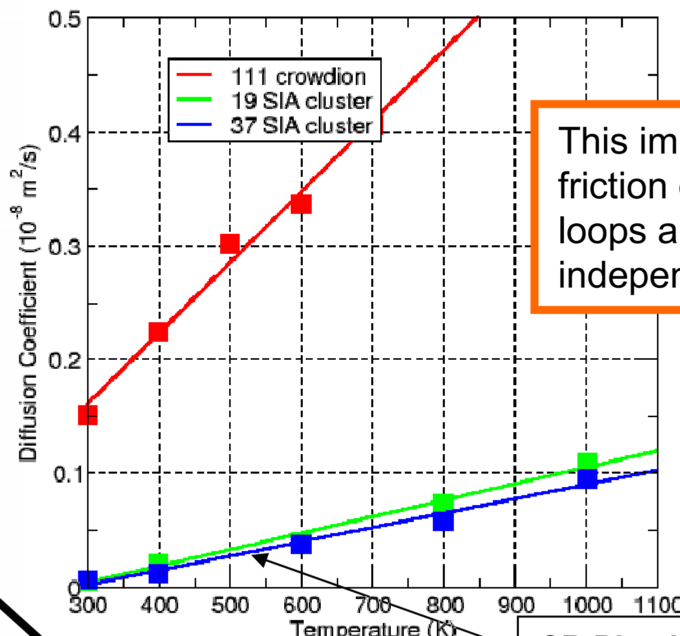
Langevin treatment of thermal drag

$$D(T) = \lim_{t\to\infty}\left[\langle x^2(t)\rangle / 2t\right] = \frac{k_B T}{\gamma(T)}$$

This is an exact equation.

If the diffusion coefficient is a linear function of T, then γ is constant.





This implies that the friction coefficient for loops and defects is independent of T.

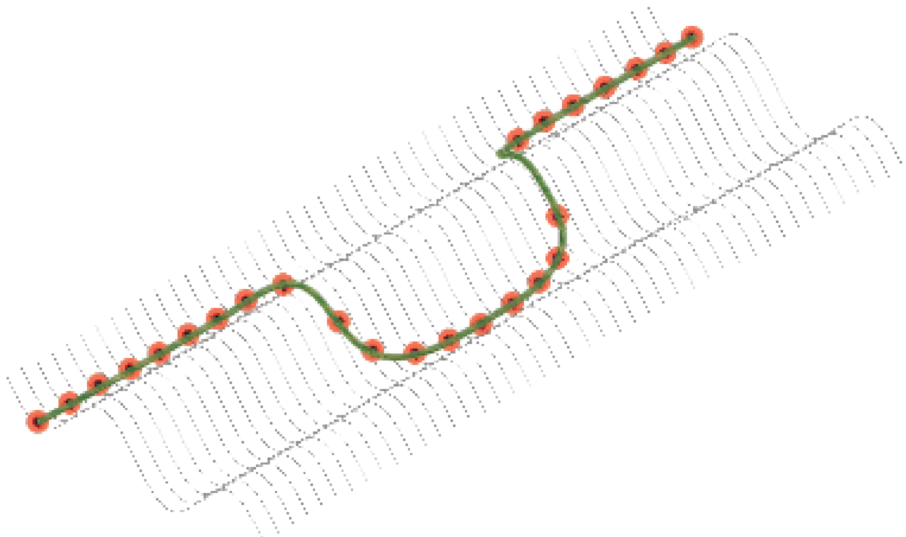
CR Physique 9 (2008) 409

P.M. Derlet et al., PRB84 (2011) 134109

Kinks on screw dislocations

Kinks on screw dislocations

$$L=\sum_{n=-\infty}^{\infty}\frac{m\dot{u}^2}{2}-a\frac{\kappa}{2}\sum_{n=-\infty}^{\infty}(u_{n+1}-u_n)^2-aE_p\sum_{n=-\infty}^{\infty}\sin^2\left(\frac{\pi u_n}{L_p}\right)$$



Field of atomic displacements in a kink

$$u(z,t)=\frac{2L_p}{\pi}\arctan\left[\exp\left(-\frac{2\pi}{L_p}\sqrt{\frac{E_p}{2\kappa}}(z-Vt)\right)\right]$$

Energy density in a kink

$$\frac{dE}{dz}=\frac{2E_p}{\cosh^2\left(\frac{\pi}{L_p}\sqrt{\frac{2E_p}{\kappa}}(z-Vt)\right)}$$

Total energy of a kink: $E_{tot}=\frac{2}{\pi}L_p\sqrt{2\kappa E_p}$

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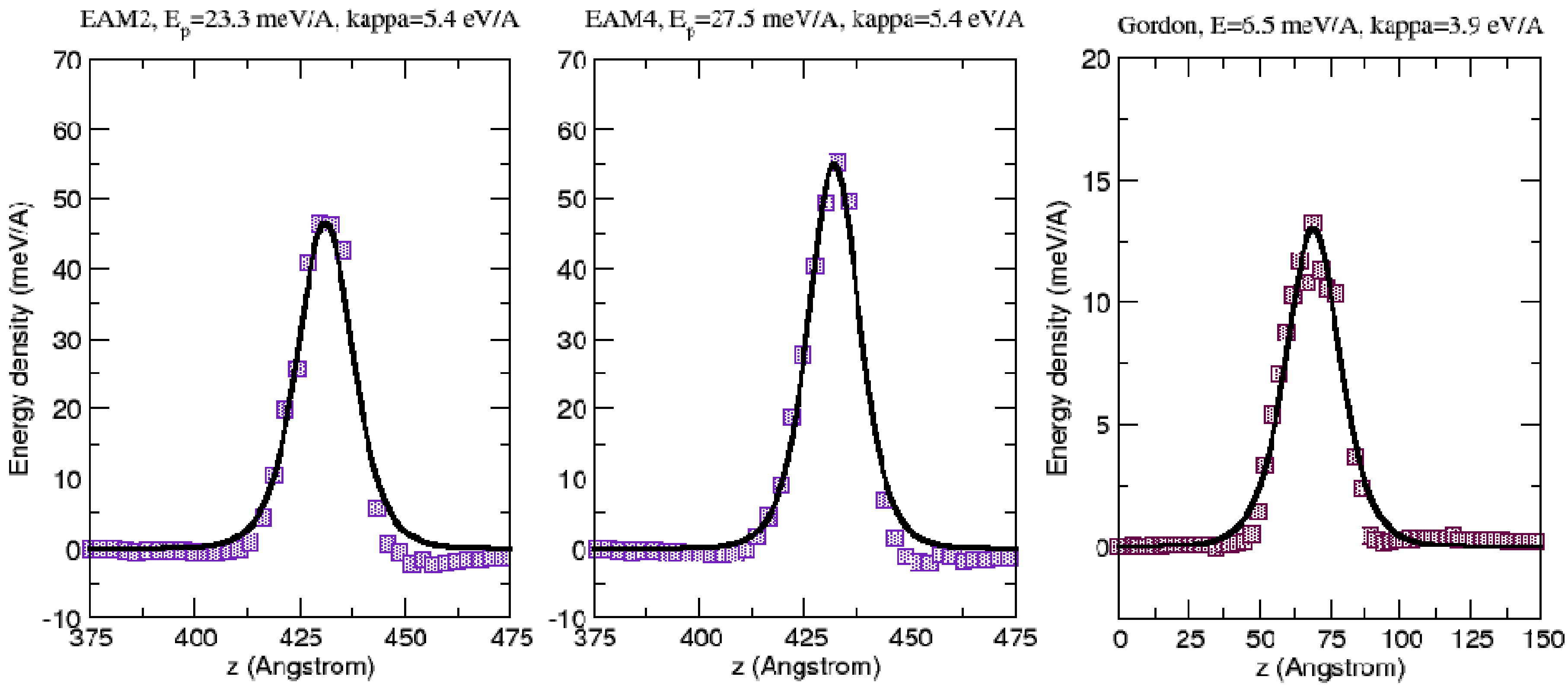
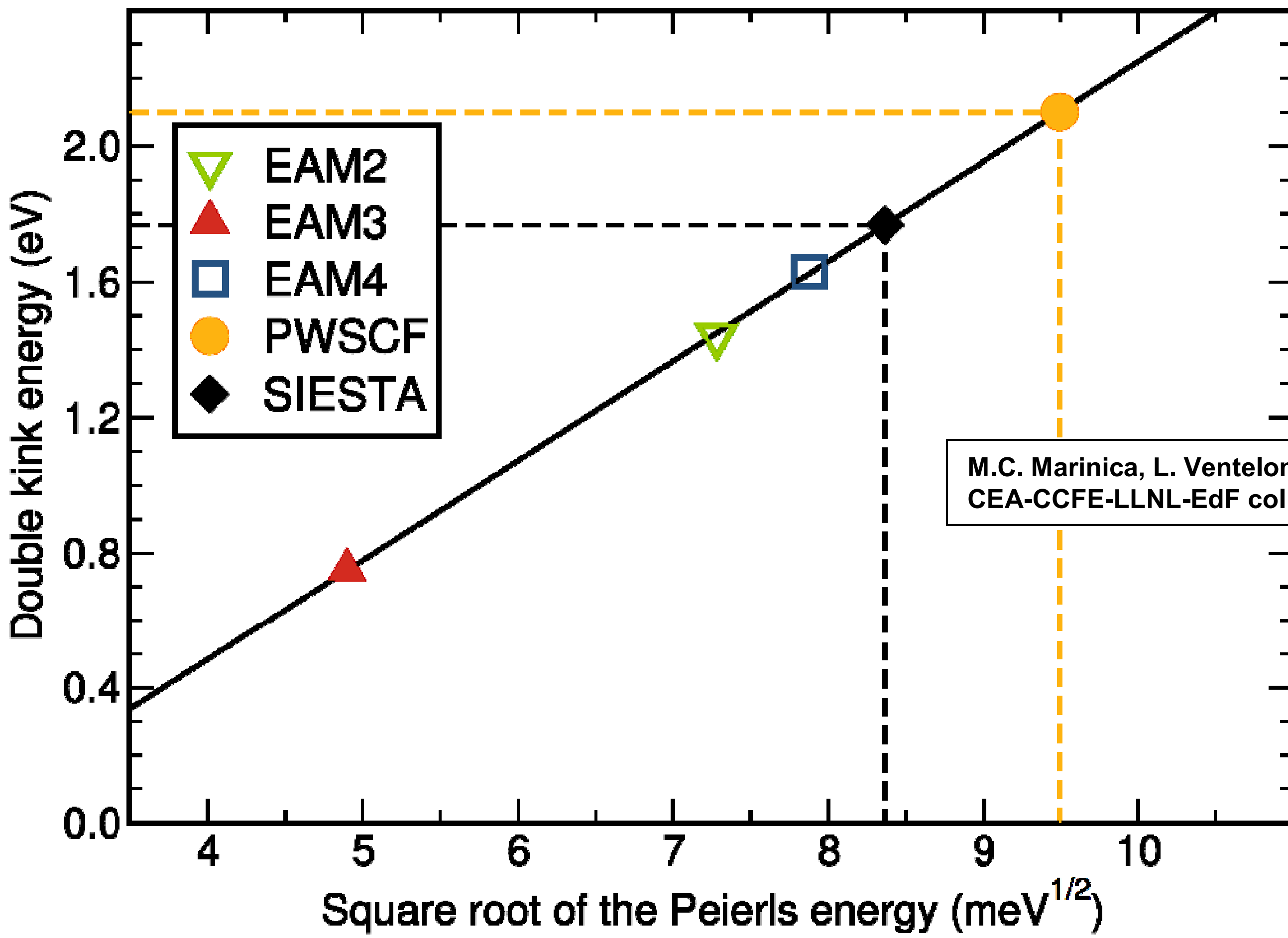
T. Swinburne *et al*. PRB 87, 064108 (2013)

Kinks on screw dislocations



Energy density in the kinks as well as their total energies are well described by the Frenkel-Kontorova model. This is the same model that was earlier, and equally successfully, applied to the treatment of crowdion defects.

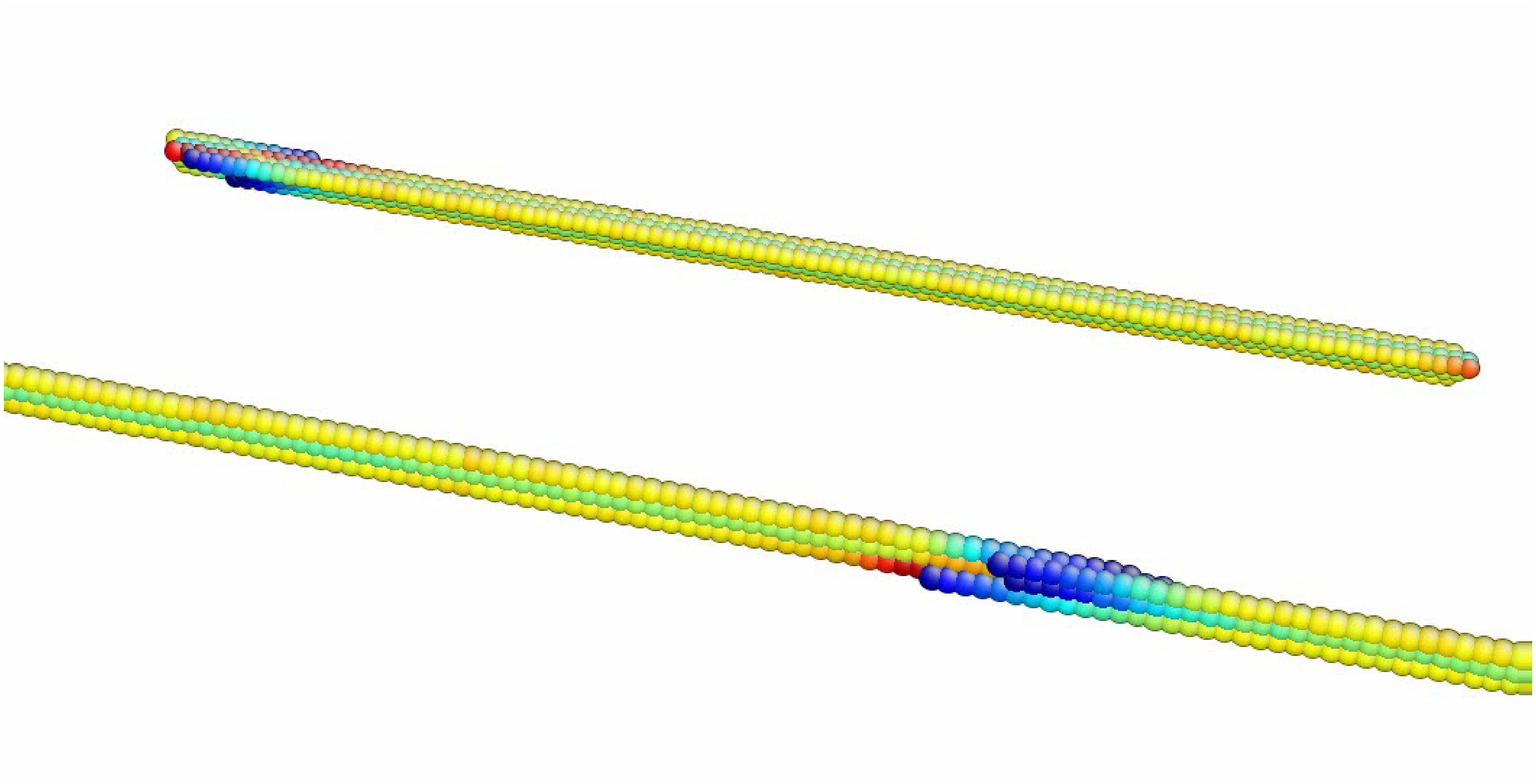
Kinks on screw dislocations



M.C. Marinica, L. Ventelon, M.R. Gilbert et al. (2013)
CEA-CCFE-LLNL-EdF collaboration

The Frenkel-Kontorova model predicts that the double kink energies should scale as the square root of the Peierls potential for the screw dislocation. This prediction is confirmed by calculations performed using three different tungsten potentials.

Thermal Brownian motion of kinks



Molecular dynamics simulations of migration of kinks on a/2<111> screw dislocations. These simulations were performed using LAMMPS and the Gordon *et al*. (2012) potential for bcc Fe, assuming T=100K, using 280x80x80b simulation box, total simulation time is 1ns.

T. Swinburne *et al*. PRB 87, 064108 (2013)

Derivation of the kink diffusion coefficient

To simulate diffusion of kinks it is necessary to use a simulation cell containing two dislocations, hence in principle there is a problem associated with interaction between kinks. The bare friction coefficient can still be derived from the data. Equations of motion for the kinks:

$$\frac{dz_1}{dt} = -\frac{D_1}{k_B T}\frac{\partial U}{\partial z_1} + \sqrt{2D_1}\xi_1(t), \quad \langle \xi_1(t)\xi_1(t')\rangle_T = \delta(t-t');$$

$$\frac{dz_2}{dt} = -\frac{D_2}{k_B T}\frac{\partial U}{\partial z_2} + \sqrt{2D_2}\xi_2(t), \quad \langle \xi_2(t)\xi_2(t')\rangle_T = \delta(t-t')$$

Introduce two new independent (also stochastic!) variables

$$z(t) = z_1(t) - z_2(t); \quad Z(t) = \left(D_2 z_1 + D_1 z_2\right)/\left(D_1 + D_2\right)$$

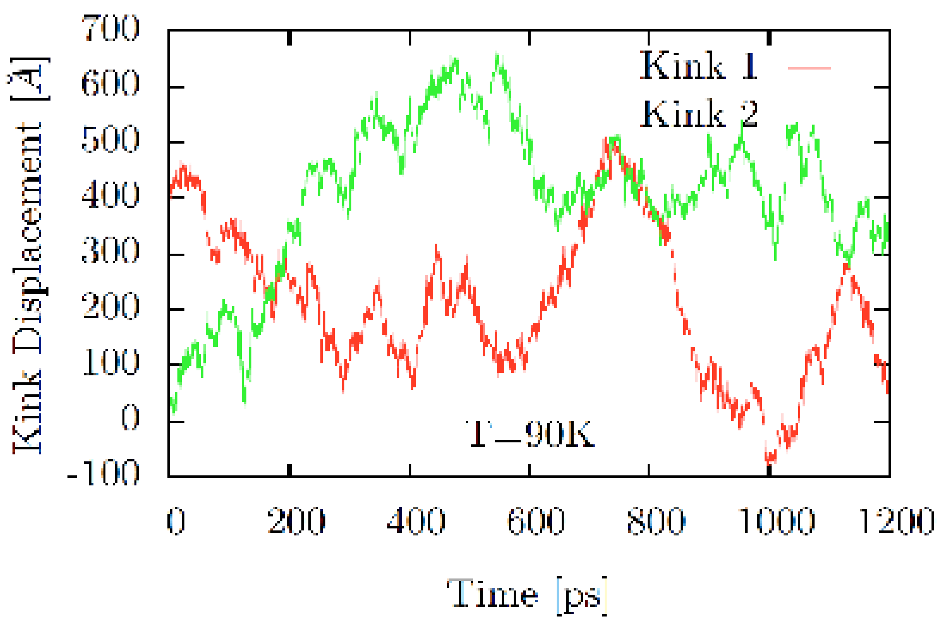
Equation of motion for the "centre of mass" (or "centre of diffusion") is <u>independent</u> of the kink-kink interaction law

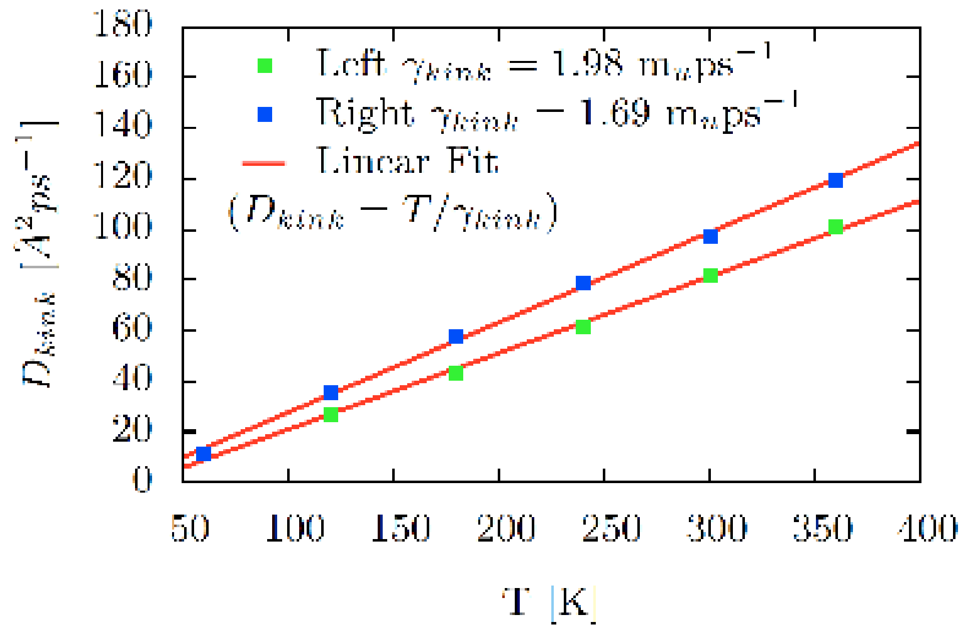
$$\frac{dZ}{dt} = \sqrt{2\frac{D_1 D_2}{D_1 + D_2}}\xi(t), \quad \langle \xi(t)\xi(t')\rangle_T = \delta(t-t').$$

Phys. Rev. B81 (2010) 224107

Brownian motion of kinks on screw dislocations in iron

It is often assumed that the friction coefficient for the kinks obeys the Liebfried law. Direct MD simulations of thermal diffusion of kinks show that the friction coefficient is <u>independent of temperature</u>, just like the friction coefficient for nano-scale defects and nano-scale prismatic dislocation loops.





D is a linear function of T

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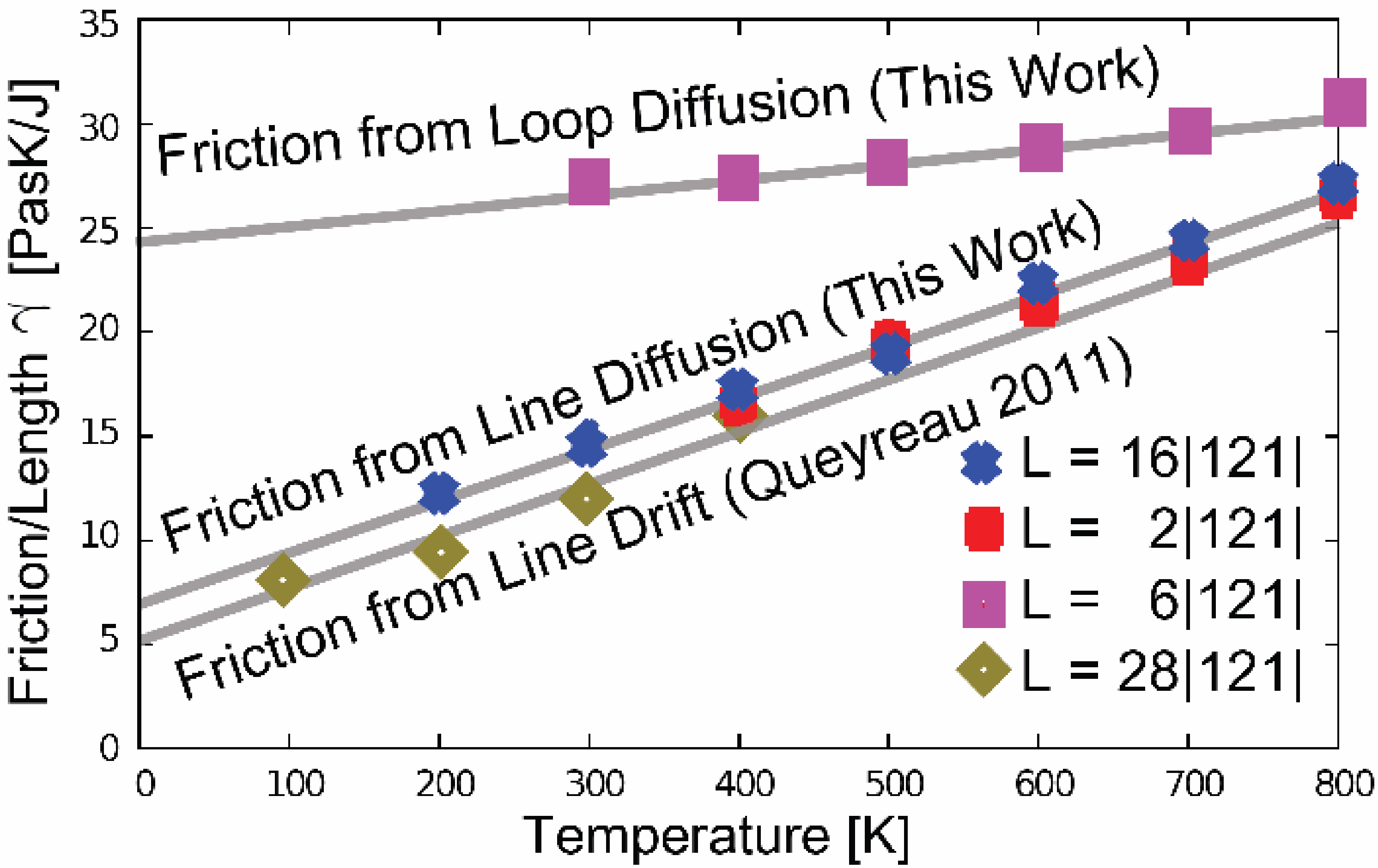
Conclusions



a/2<111>{110} edge dislocation lines and loops.

T. Swinburne *et al*. PRB 87, 064108 (2013)

Conclusions

$$\gamma(T) = A_{wind}T + B_{origin \quad unknown}$$

There is a significant T-independent contribution to drag, the origin of which is unknown, which is dominant for nano-scale defects and kinks.

Motion of line dislocations is almost unaffected by the anomalous T-independent term.

Bridging MD and DDD on the nanoscale appears problematic.