Using Defects to Store Energy

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Outline

Windscale Fire

Worst Nuclear Disaster in Great Britain's History

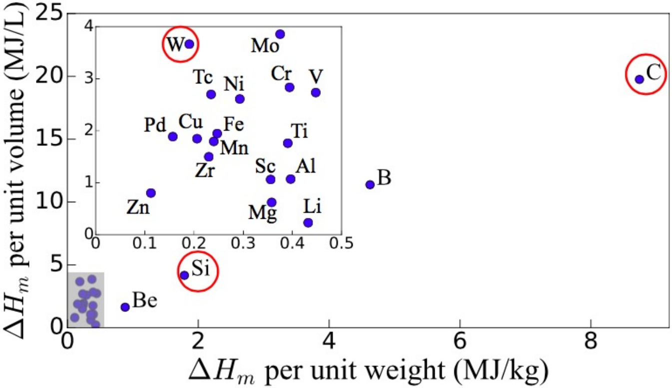
- October 10, 1957.
  Northwest England.
- Fire burnt for three days.
- *Wigner Energy*

Rationale

- Defects have an energy cost.
- Non-equilibrium defects.
- Long-lived. Stable at Room Temperature.

Proof?

Setting up the Calculations



ΔH_m gives the upper limit.

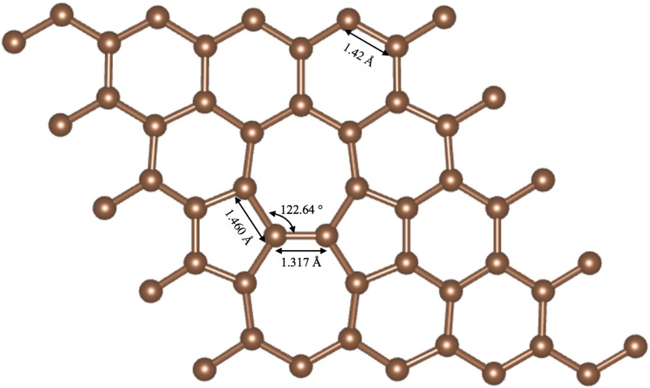
Setting up the Calculations

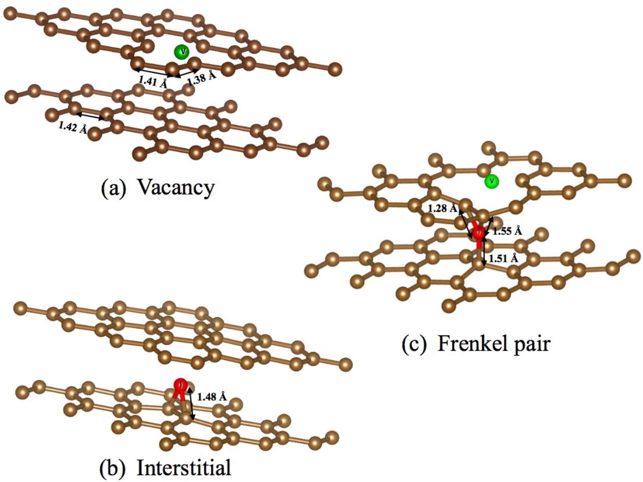
Materials

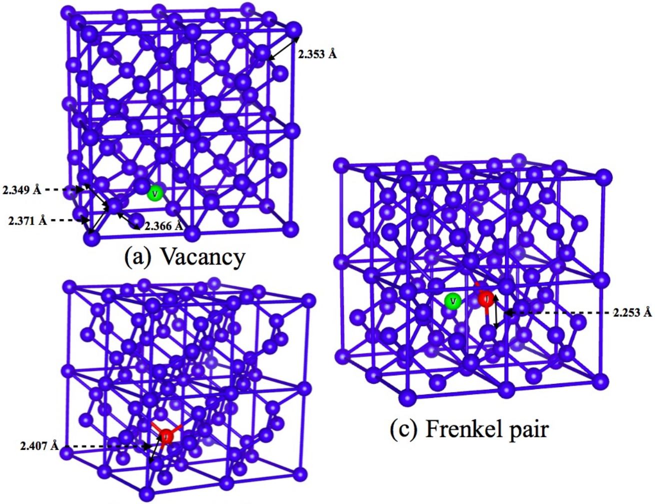
- Graphite, Graphene, Diamond
- Si
- W

Defects

- Vacancies
- Interstitials
- Frenkel Pairs
- Stone-Wales Defects


1.42 Å
122.64 °
1.460 Å
1.317 Å

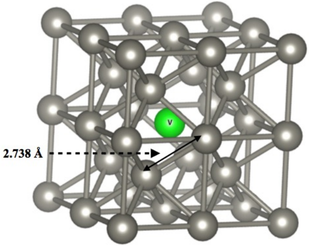

1.41 Å
1.38 Å
1.42 Å
(a) Vacancy
1.28 Å
1.55 Å
1.51 Å
(c) Frenkel pair
1.48 Å
(b) Interstitial



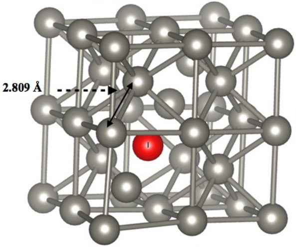
(a) Vacancy

(b) Interstitial

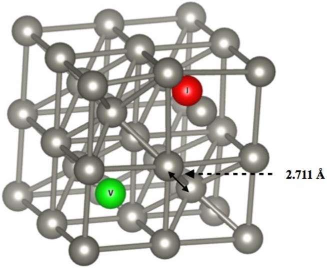
(c) Frenkel pair



(a) Vacancy



(b) Interstitial



(c) Frenkel pair

Calculation Methods I

Defect Formation Energy

$$E_F = E_D - \left(\frac{N}{N_0}\right) \times E_0$$

E_F - Defect Formation Energy

E_0 - Energy of Pristine Cell (N_0 atoms, 0 defects)

E_D - Energy of Supercell (N atoms, 1 defect)

Bigger the N, better the estimate.

Calculation Methods II

Stored Energy

$E = E_F \times C_{NE}$

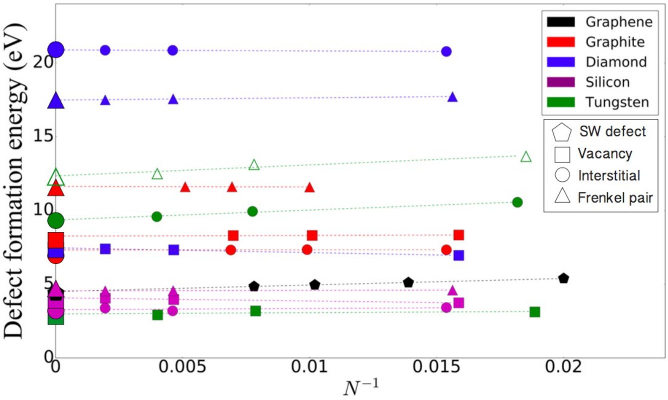
E - Energy stored

E_F - Defect Formation Energy

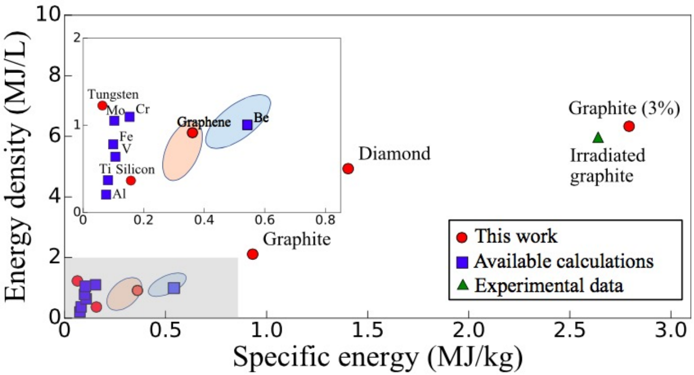
C_{NE} - Concentration of non-equilibrium defects

$C_{NE} \sim 1$ at.%

Calculated E_F

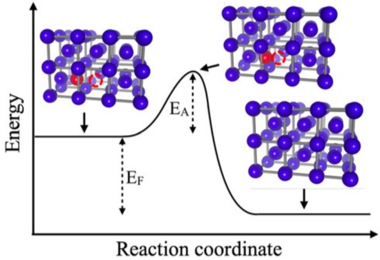


Calculated E



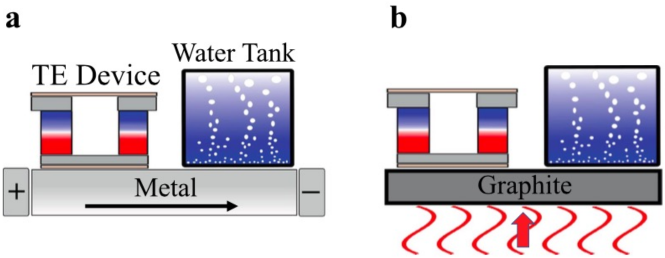
Works!

Role of Kinetics



- This energy is *borrowed* and will be returned.
- Conventional may be inefficient. Localised is better.
- Positive feedback possible.

Proof of Concept



- Storage Efficiency (η_S).

$$\eta_S = \frac{formation}{generation}$$

- Release Efficiency (η_R).

$$\eta_R = \frac{stored + input}{input}$$

Main Challenges

- Simple and inexpensive ways to generate defects.
- Minimal waste during recombination.
- Mechanically and chemically stable materials during generation and recombination.
- Reversible storing and releasing of energy.
- Defect aggregation during release.

We don't want another Windscale!

Denouement

- Follows an emerging trend : *Cis-Trans Azobenzene*
- Generalises the idea of energy storage using bond rearrangement.
- Niche Applications
  - Heating, Catalysts
  - Combustion
  - Space-shuttles

    Infinite Improbability Drive?

Summary

- Storing energy using defects is a novel idea.
- Calculations show promising results.
- Engineering is an open challenge.

- Outlook
  - High-throughput calculations to identify better materials.
  - Practical implementation.

Further Reading

Lu, I-Te and Bernardi, Marco.
Using defects to store energy in materials - a computational study
Scientific Reports, 2017.

Matlack, Gerry.
The Windscale Disaster
Damn Interesting, 2007.
https://www.damninteresting.com/the-windscale-disaster/