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Paul Scherrer Institut
Jiachao Chen

A New Mechanism of Loop Formation and Transformation in bcc Iron without Dislocation Reaction

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Contributors:

J. Chen[1], N. Gao[1, 2], P. Jung[1], T. Sauvage[3]

[1]Department of Nuclear Energy and Safety, Paul Scherrer Institut,
CH-5232 Villigen PSI, Switzerland
[2]Institute of Modern Physics, Chinese Academy of Science,
73000 Lanzhou, P.R. China
[3]CEMHTI/CNRS, Université d'Orléans, 3A rue de la Férollerie,
45071 Orléans CEDEX 2, France

Outline

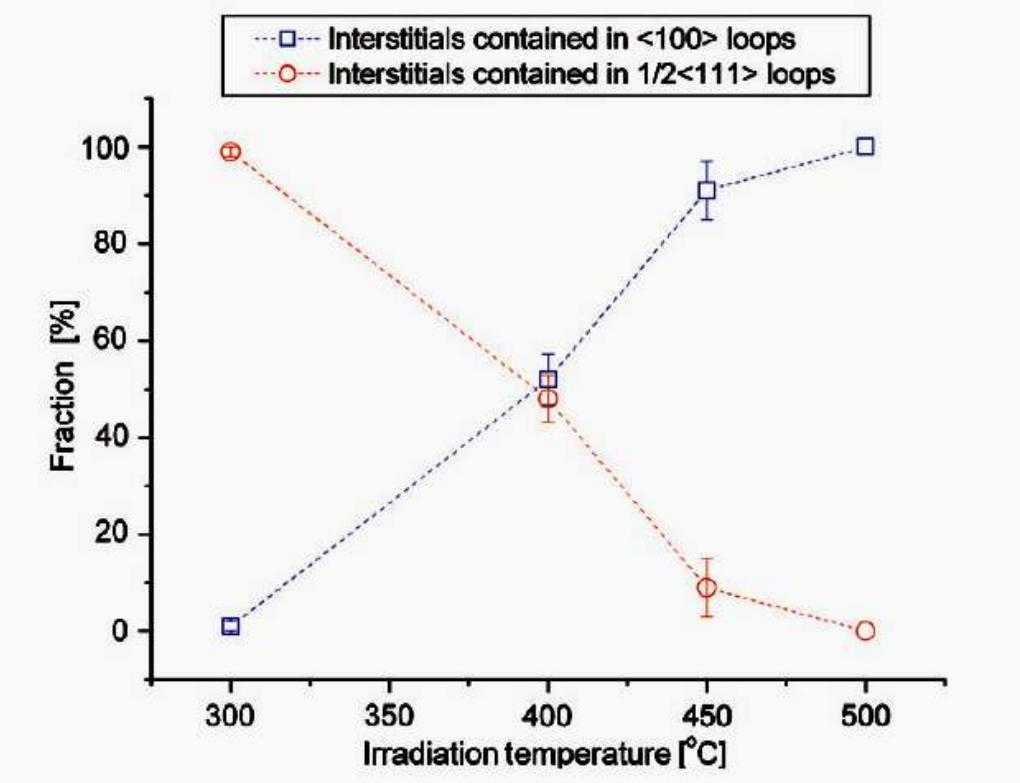
1. **Introduction**
2. Experimental Evidence
3. Proposed Mechanism
4. MD simulation and discussion
5. Conclusion

Dislocation loops formed by irradiation damage in Fe-Cr alloys

Coexistence of ½<111> and <100> loops

Configurations:

b	½<111>	<100>
habit planes	{111} {110}	{100}
nature	I	I



Z. Yao, et al. Philosophical Magazine, Vol. 90 (2010) 4623

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Previously proposed mechanisms for formation/transformation of 1/2<111> and <100> loops in Fe-Cr alloys

Eyre and Bullough
[Philos.Mag. 12 (1965) 31]

$$\tfrac{1}{2}[110] + \tfrac{1}{2}[00\bar{1}] \rightarrow \tfrac{1}{2}[11\bar{1}]$$
$$\tfrac{1}{2}[110] + \tfrac{1}{2}[\bar{1}10] \rightarrow [010].$$

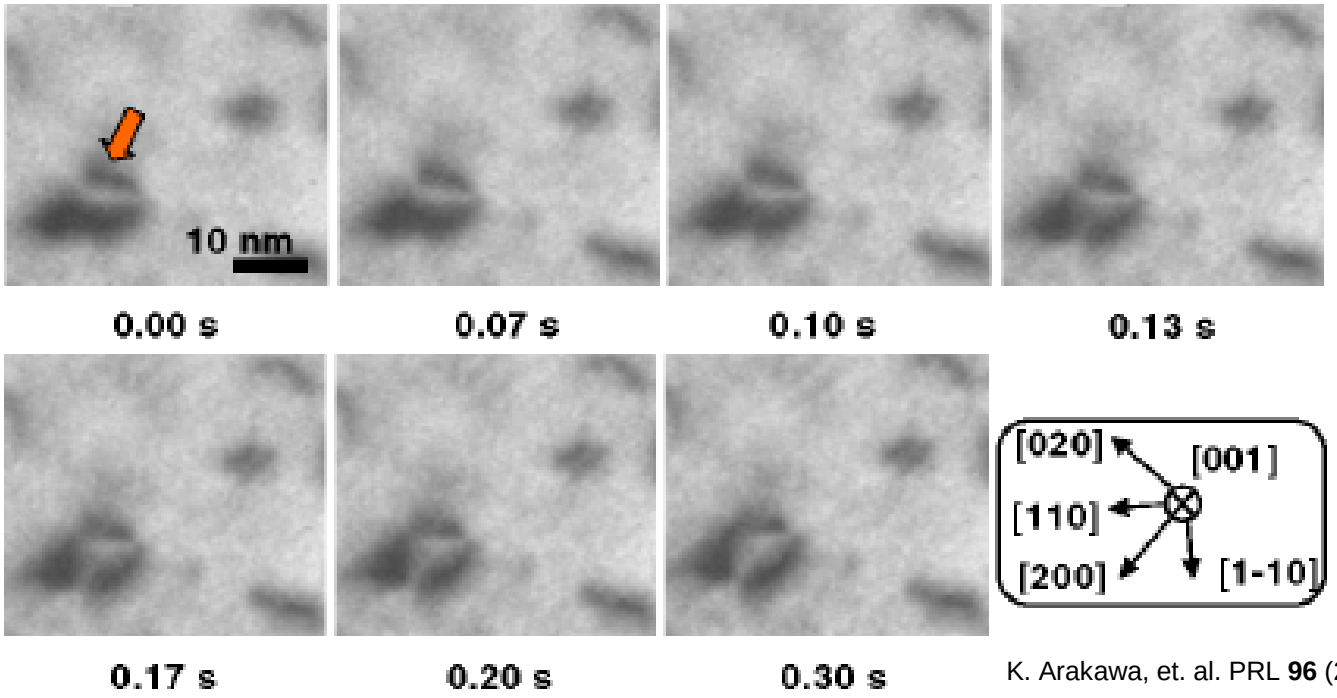
Marian et al.
[PRL 88 (2002) 255507-1]

$$\tfrac{1}{2}[111] + \tfrac{1}{2}[00\bar{1}] \rightarrow \tfrac{1}{2}[110],$$
$$\tfrac{1}{2}[110] + \tfrac{1}{2}[1\bar{1}0] \rightarrow [100].$$

B. C. Masters
[Philos. Mag. 11 (1965) 881]

$$\tfrac{1}{2}[111] + \tfrac{1}{2}[1\bar{1}\bar{1}] \rightarrow [100]$$

Contradiction to recent experiments



Change of loop Burgers vectors from ½<111> to <100> and vice versa without loop/dislocation interaction

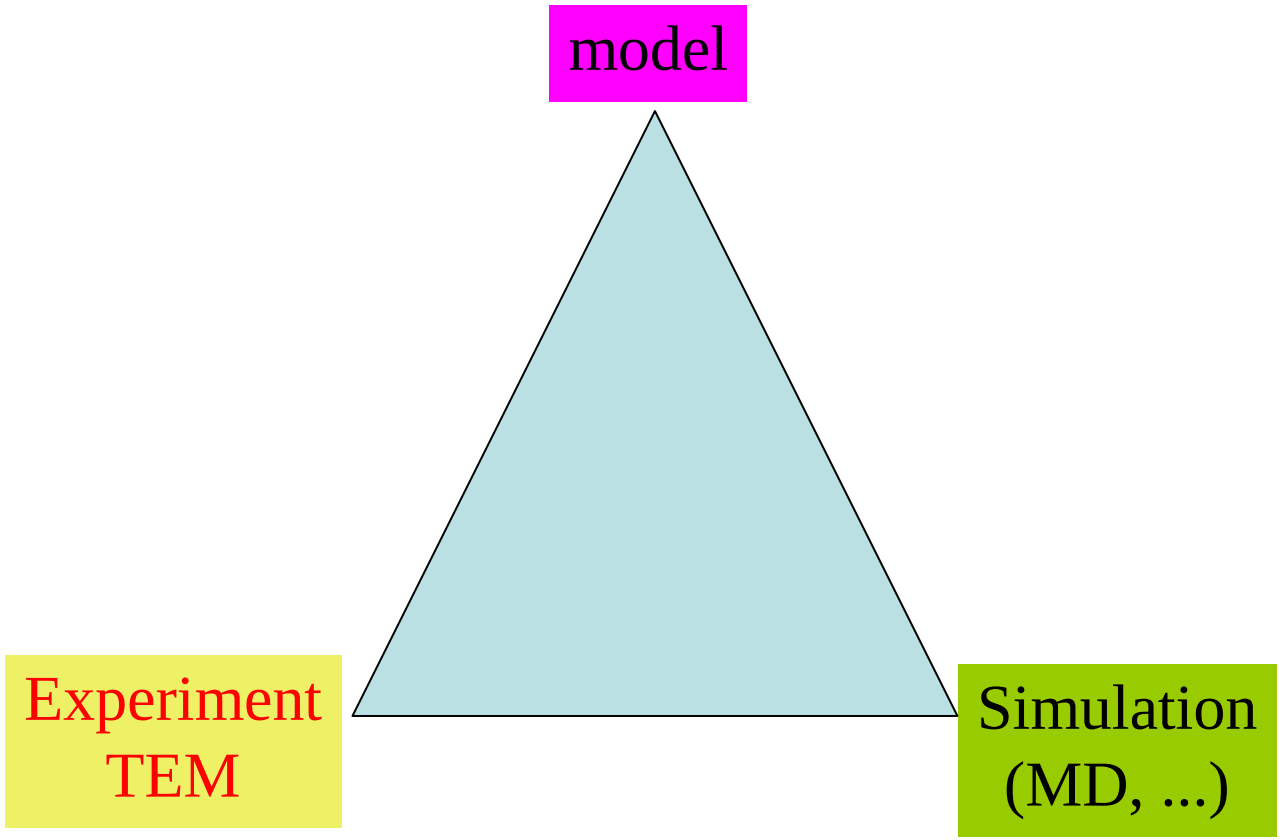
K. Arakawa, et. al. PRL **96** (2006) 125506

In another experiment: K. Arakawa, T. Amino, H. Mori, Acta Mater. 59 (2011) 141

large loops absorb small ones with different b by an absorption reaction without changing its own b.

This is also realized in MD simulation.

Study methods



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Experimental details

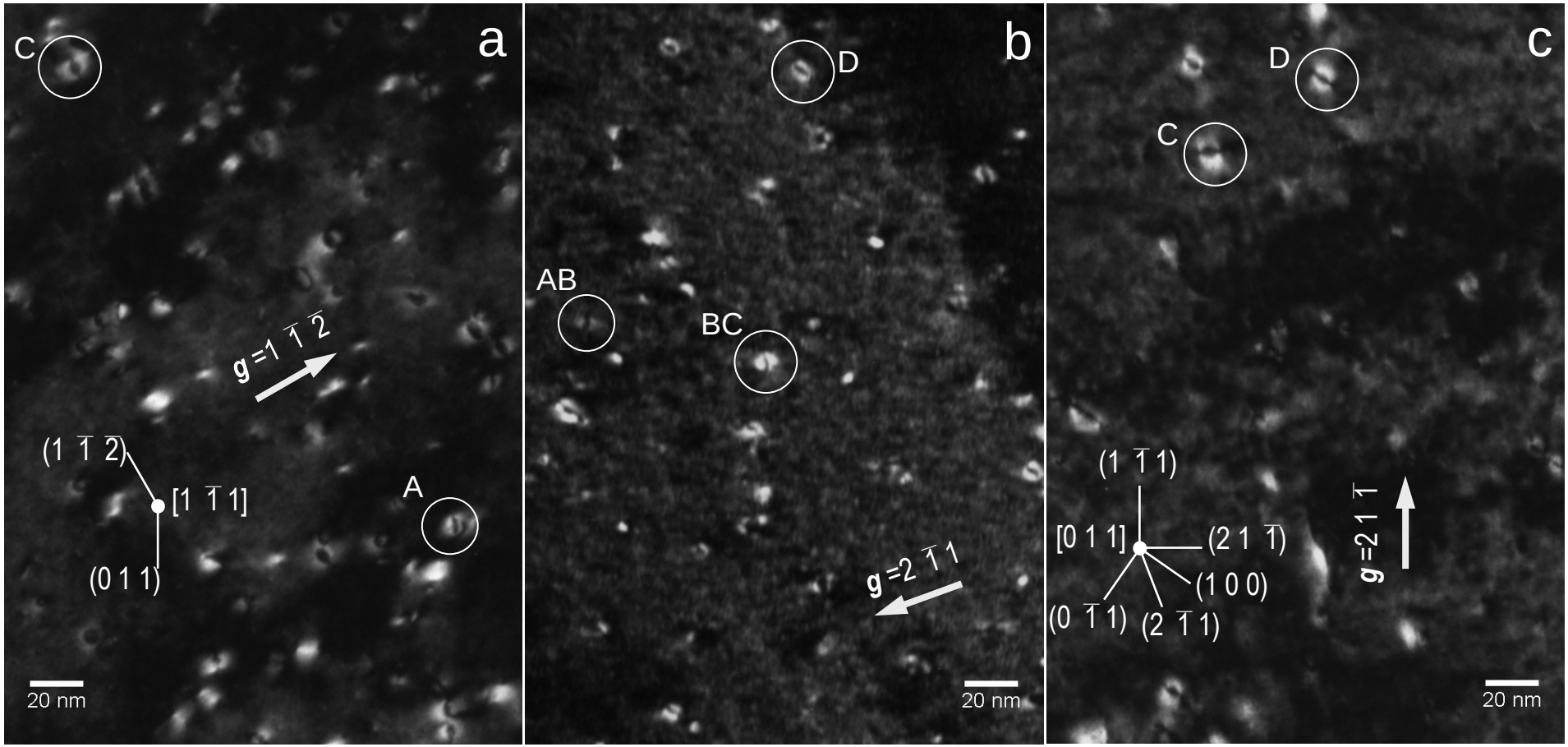
Materials:

polycrystalline Fe (99.99+%), supplied by Goodfellow

Experiments Performed:

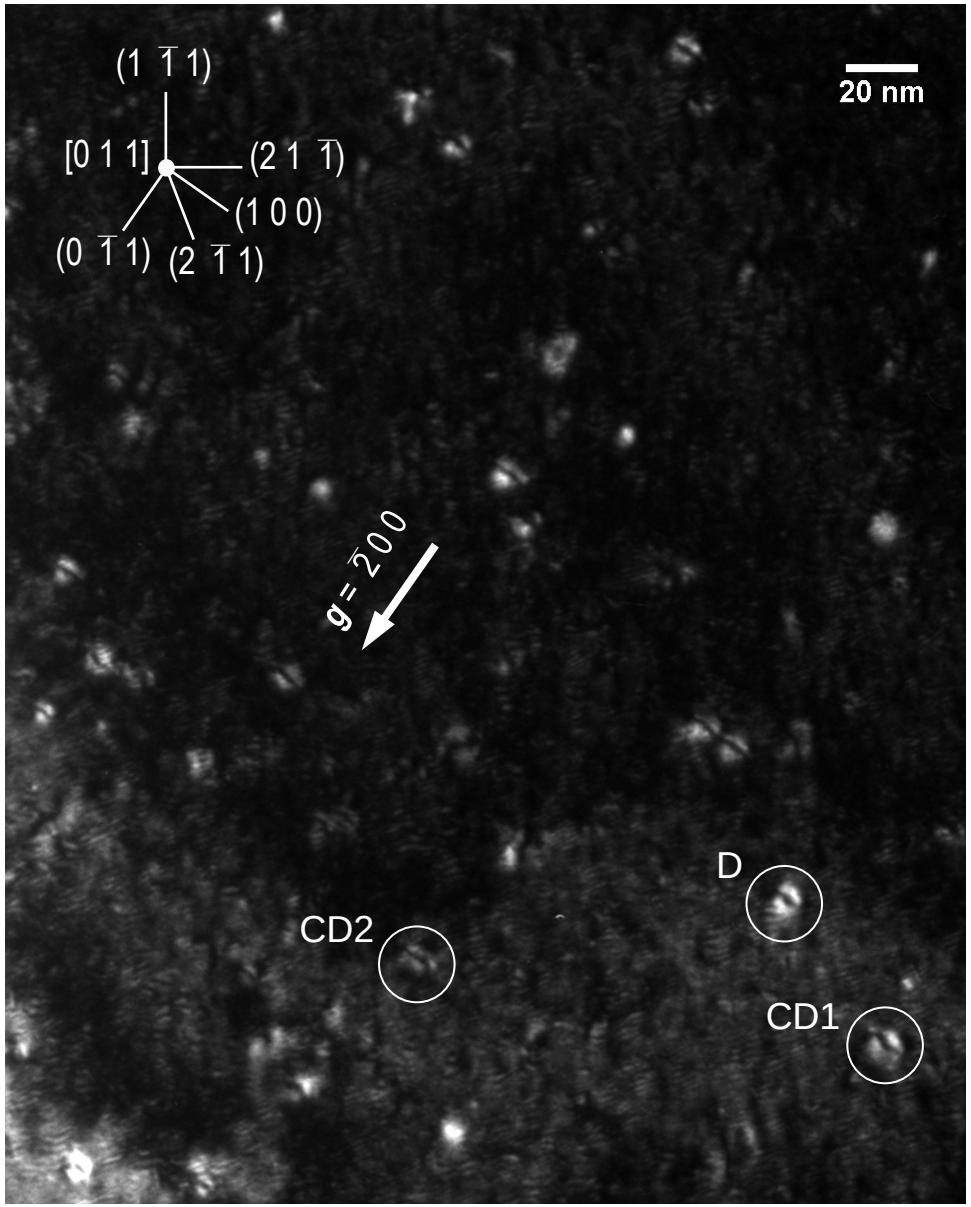
- Specimens of 0.1 mm thick annealed isothermally at 1073 K for 1 hour
- 3D-homogeneous Irradiation/implantation with 25 MeV α-particles up to 0.13 dpa with damage rate of 5.4×10^{-6} dpa/s at 573 K
- 1 mm diameter discs technique is used for TEM sample preparation
- Loop was analyzed by edge-on view and standard $\boldsymbol{g \cdot b}$ techniques

Loops in iron after irradiation at 573K to 0.13 dpa



Loops "A", "B", "C" and "D" have the configuration of ½<111>{110}, ½<111>{111}, ½<111>{211} and <100>{100}, respectively, double-letter loops have composite habit planes, e.g. "AB": (0$\underline{1}$1)+(1$\underline{1}$1), "BC": (1$\underline{1}$1)+(2$\underline{1}$1). Edge-on loops in Fig. a have habit planes (11 $\underline{2}$) and (011), in Fig. b+c: (0$\underline{1}$1), (1$\underline{1}$1), (2$\underline{1}$1), ($\underline{1}$00), (21$\underline{1}$), and (11$\underline{1}$).

Loops in iron after irradiation at 573K to 0.13 dpa



Loops composed of ½<111>{2$\underline{1}$1} and <100>{100} components are marked by “CD1” and “CD2”.

loops “AB” and “BC” — visible in Fig.b; disappear in Fig. c → ***b***= ½[11$\underline{1}$],

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loop “C” — visible in fig. c; disappears in fig.1b, → ***b***= ½[1$\underline{1}$1].

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similarly, the loop “D” in fig. b+c, is identified as type <100>(100).

In summary, the loop configuration appearing in the specimen are:

A: ½<111>{110}, B: ½<111>{111}, C: ½<111>{211}, D: <100>{100}, and their composites AB, BC and CD. The CD are considered intermediate stages in transformation from ½<111 > to <100>

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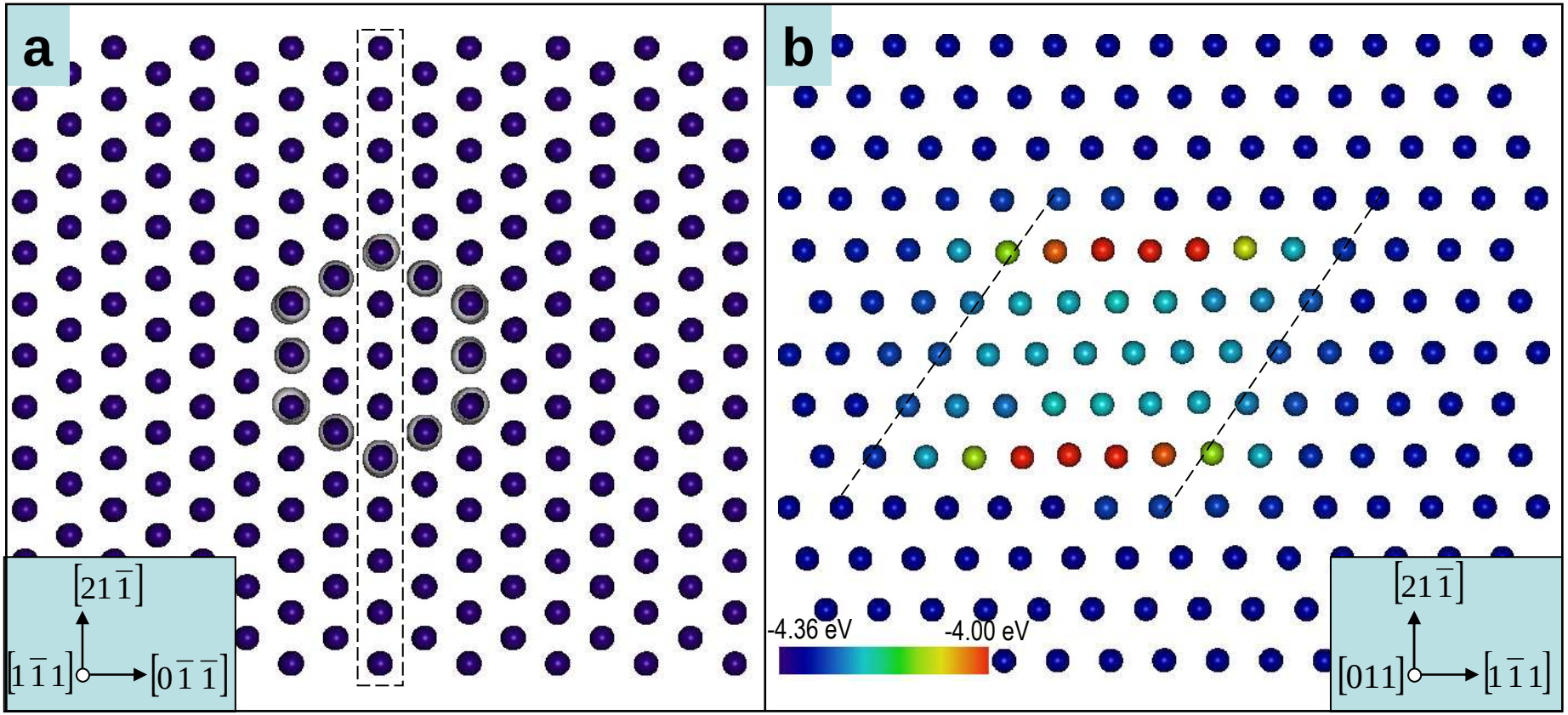
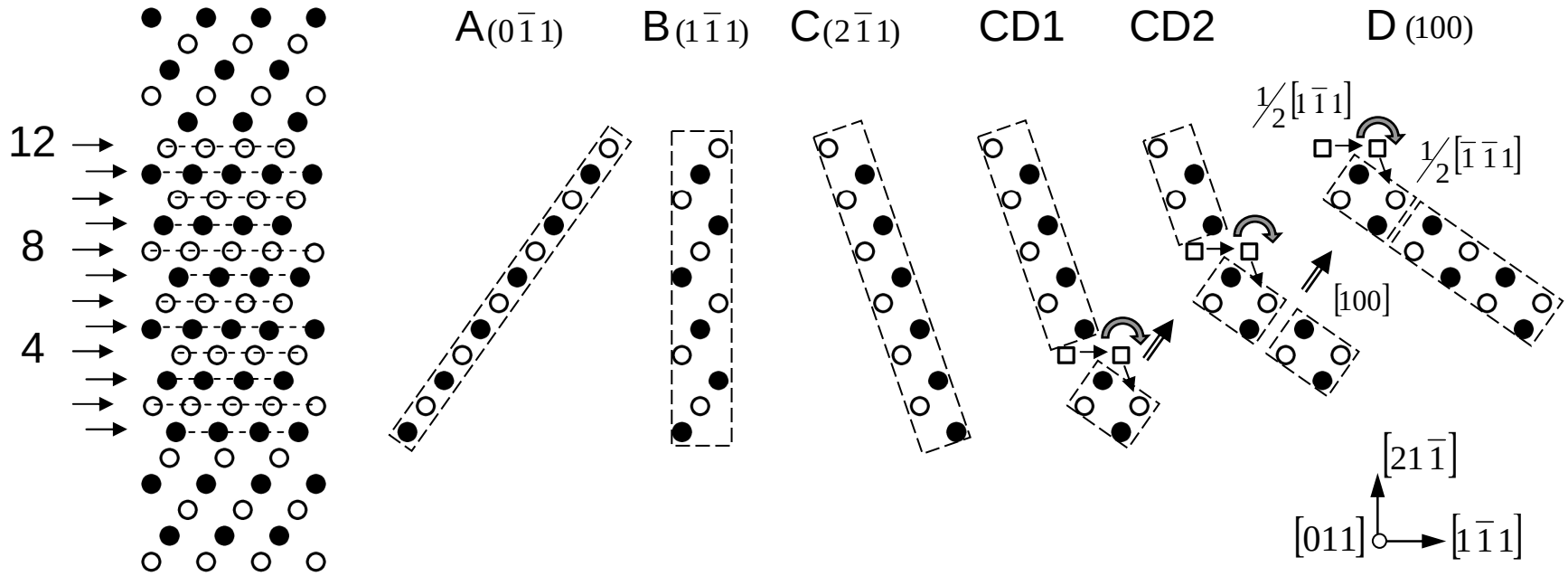
Loop formed by closely arranged parallel ½<111> crowdions



Proposed model in which the transformation steps are depicting the loops observed by TEM



In a (4+1)-step process (pathway) also a transition of a ½[1$\underline{1}$1](2$\underline{1}$1) loop to <100>(100) is possible: (1) the <1$\underline{1}$1> crowdions glide a step ½[1$\underline{1}$1]; (2) rotate from a [1$\underline{1}$1] to a [$\underline{1}$ $\underline{1}$1] crowdion; (3) the [$\underline{1}$ $\underline{1}$1] crowdions glide a step ½[$\underline{1}$ $\underline{1}$1]; (4) the SIAs jump to a [100] orientation and form segments of a <100>(100) loop; (5) a segment of the <100>(100) loop glides a step along [100]. Steps (1) to (5) are repeated until the whole loop is transformed.

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MD Simulation Parameters

Ensemble: NPT

Approach: Parrinello-Rahman algorithm, nudged elastic band method

Fe-Fe potential: Ackland [1997]; Mendelev [2003]; Dudarev-Derlet [2008]

Cell box: up to 40x15x25 cells
Loop sizes: up to 500(~ 5 nm) atoms

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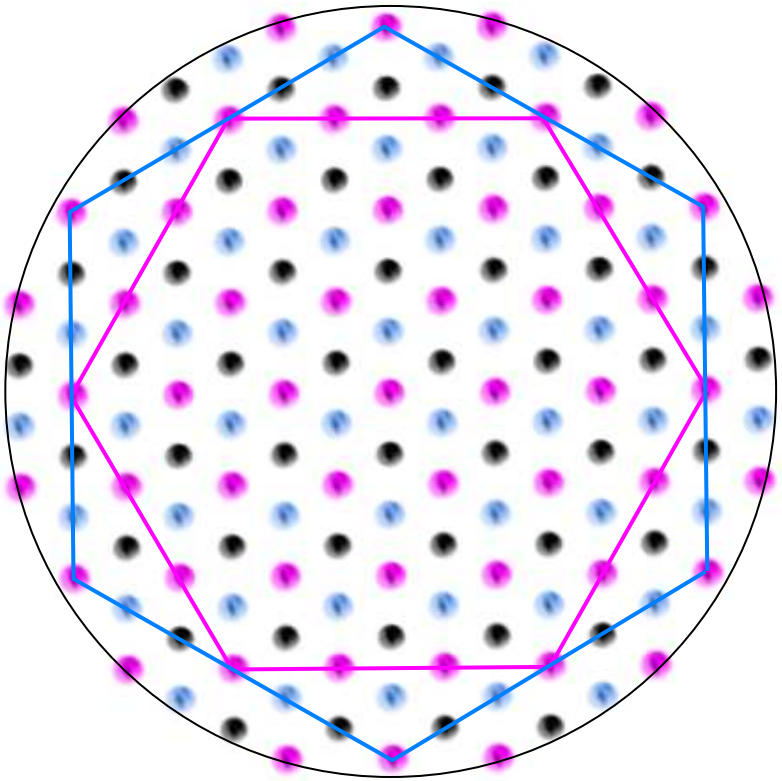
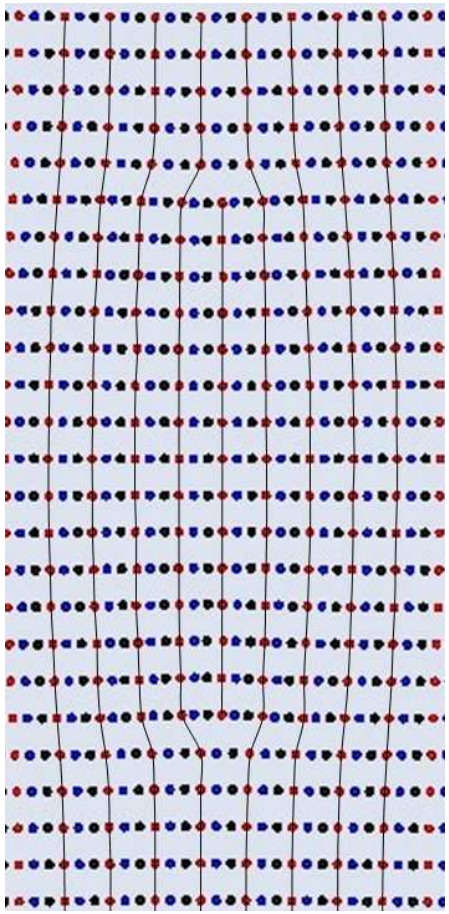
1/2⟨111⟩{111} loop

Face-on view

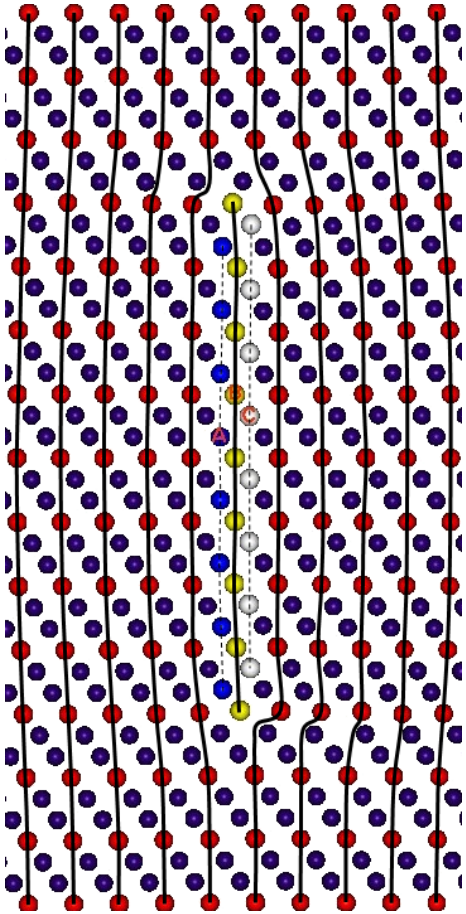


Edge-on view

Line ⟨211⟩



Line ⟨110⟩



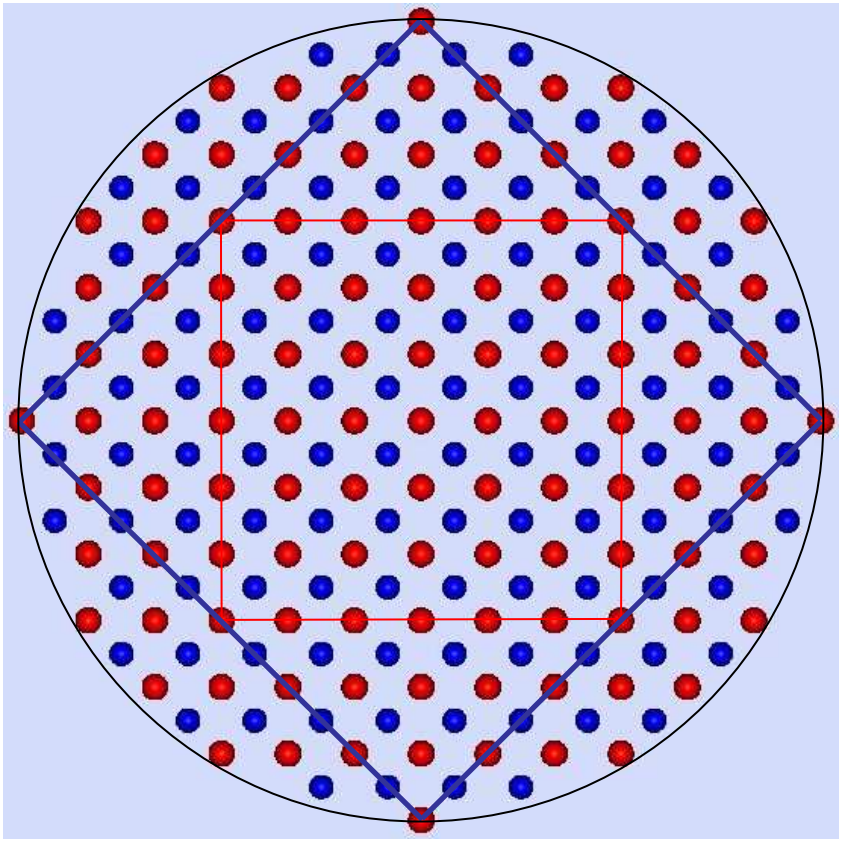
⟨100⟩{100} loop

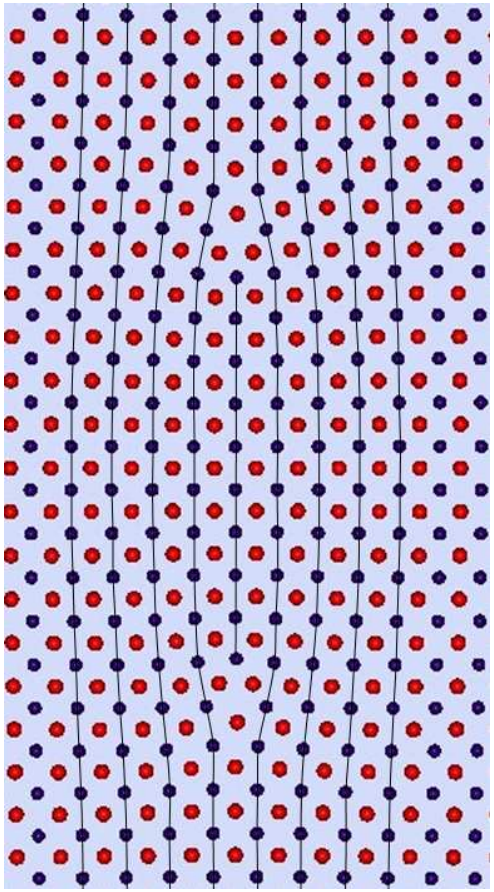
Face-on view

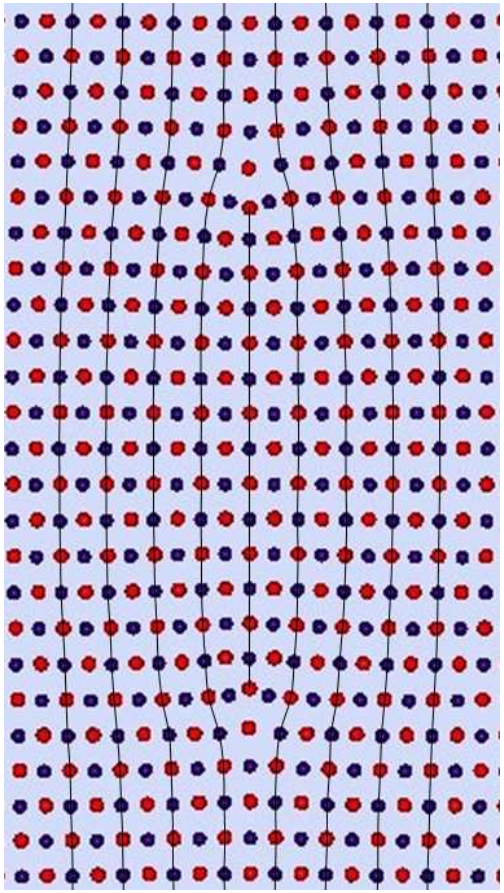
Edge-on view

Line ⟨100⟩

Line ⟨110⟩







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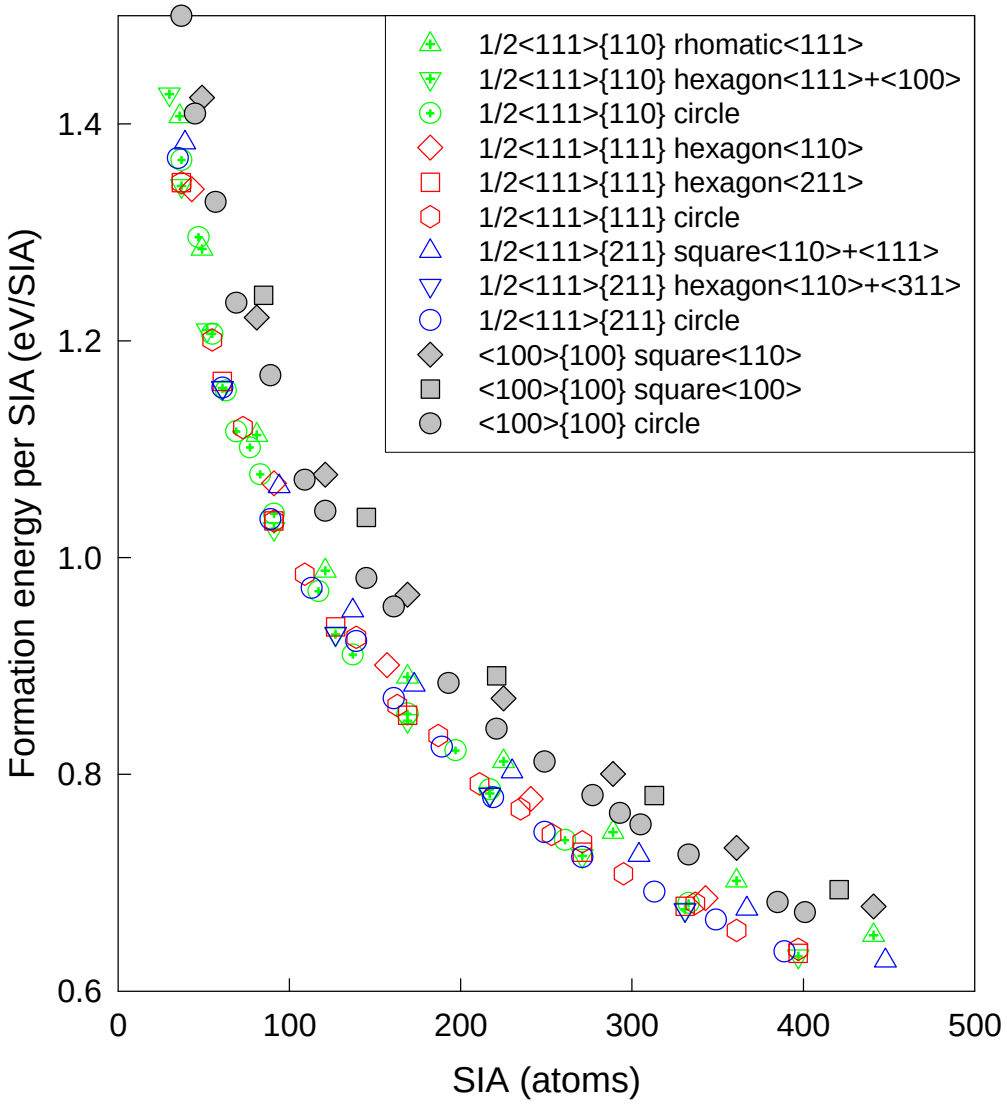
Formation energies per SIA of loops



Up to now, MD simulation with various potentials shows that 1/2[111] loops are always more stable up to 1000 K. Only the considerations on temperature dependence of elastic constants, which affect the anisotropic elastic self-energies of dislocation in iron, could account for the experimental observation of <100> loops at 573 K and the increase portion of <100>{100} loop with increasing temperature up to 773 K. To clarify this point, a new potential, valid at elevated temperatures is demanded

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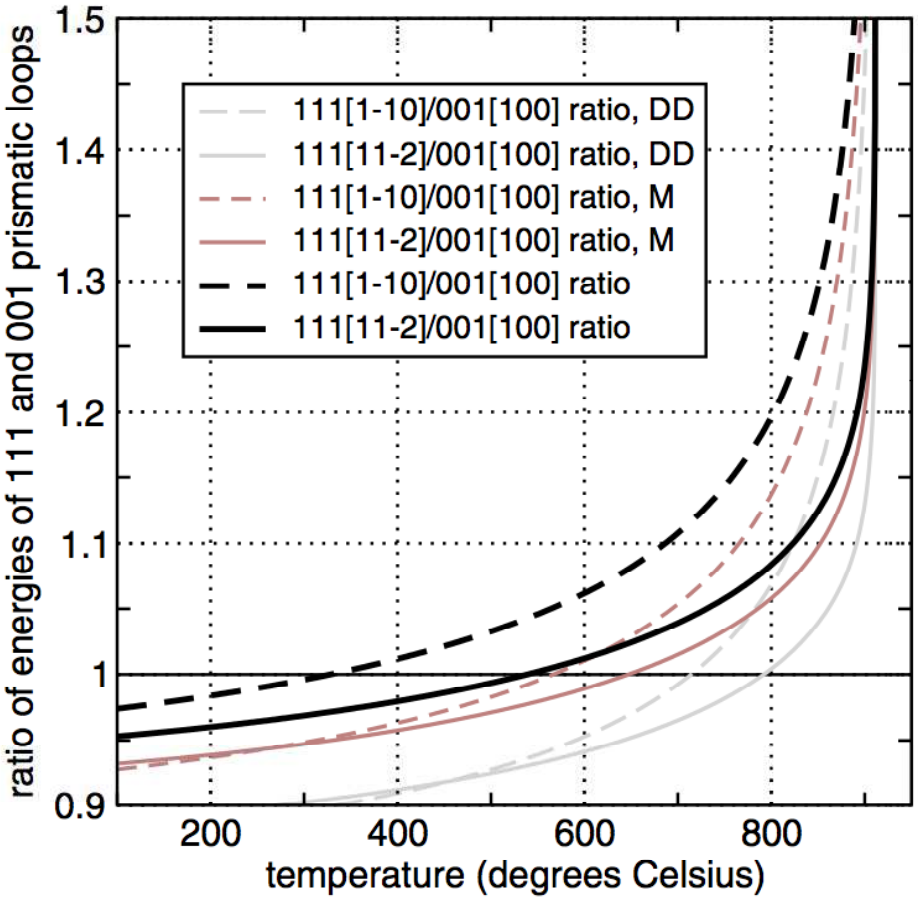
Thermodynamic reasoning

Ratio of the total free energies calculated using elasticity of the continuum of 10 nm prismatic loops with 1/2 <111> to <100> Burgers vector as a function of temperature. The two sets of lighter lines correspond to using a dislocation core energy found using the empirical potentials for α-Fe, whereas the darker curves represent the best fit of the dislocation core energy to experimental observations. The temperature dependence is the one of the elastic constants, which was measured experimentally.

S.L. Dudarev, R. Bullough and P.M. Derlet, Phys. Rev. Lett. 100(2008)135503



kinetic processes

The kinetic processes occurring in the above loop transformation
A) glide of <111> crowdions along <111>;
B) glide of segments of {100} loops along <100>;
C) jumping of <111> crowdions between different <111> directions, and rotation into <100> orientation.

The loop glides by forming and moving double kinks as described in text books. In this case, the apparent activation energy will be the sum of kink formation energy and migration energy of a dislocation segment.

The activation energy calculated by diffusivity calculation method for the ½<111> loop is in all cases less than 0.1 eV which is lower than the experimental value of roughly 0.4 eV for “naked” loops

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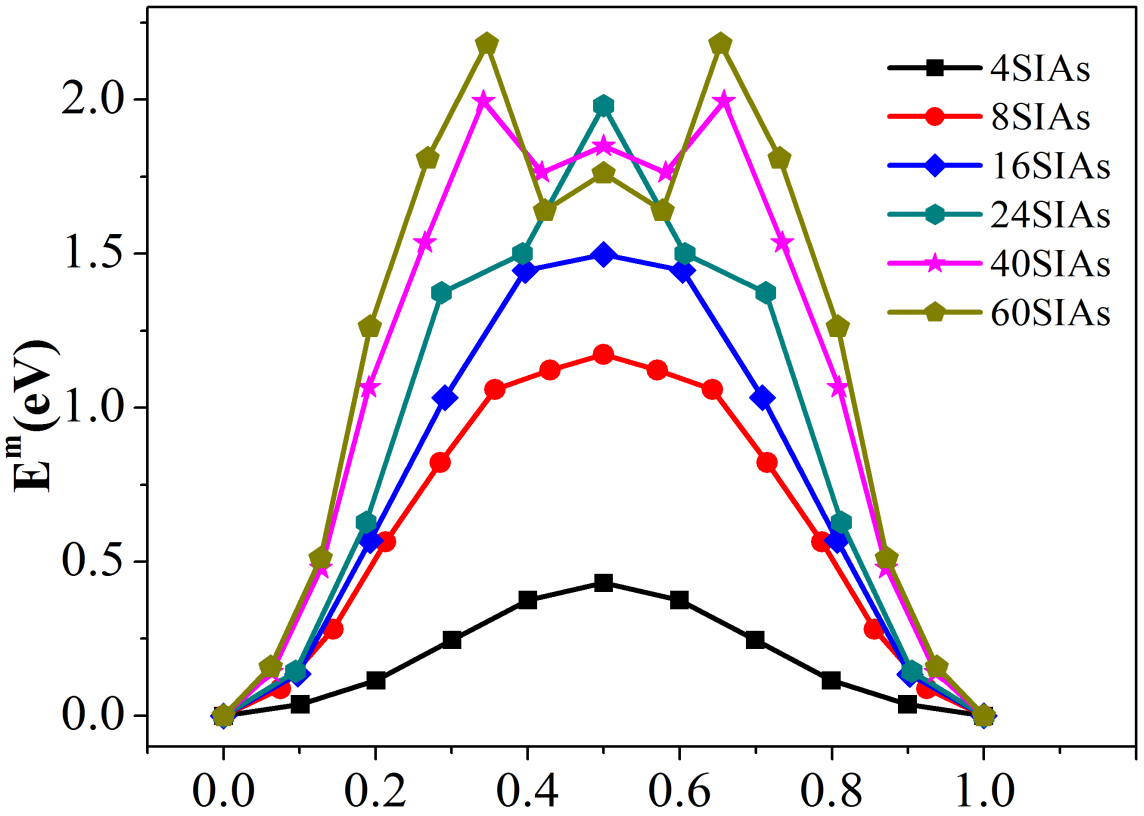
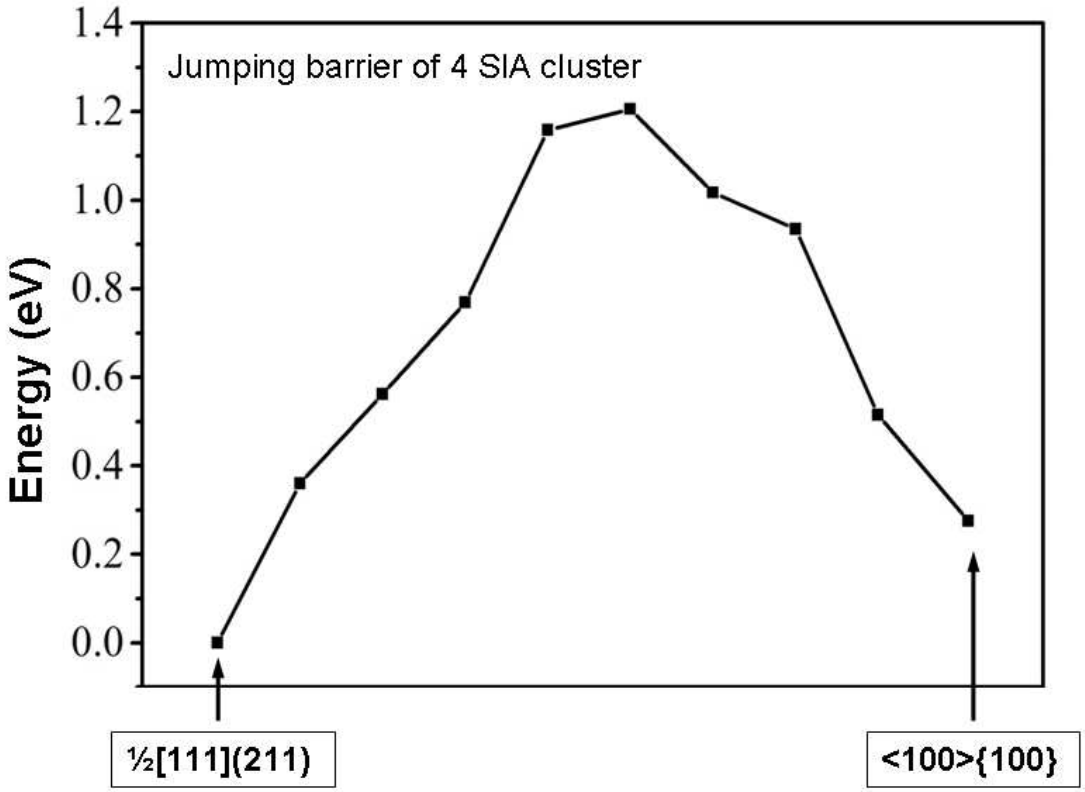
glide barrier of <100> loop



The activation energy for gliding of a loop along <100> is estimated by migration energy of a dislocation segment containing 4 SIAs (0.4 eV) plus a double kink formation energy (~0.5 eV) resulting ~0.9 eV.

Reorientation barrier of SIA cluster



The energy barrier for an isolated 4 SIA cluster jumping from a <111> crowdion arrangement to a <100> orientation via the proposed pathway resulting in a minimum size of a meta-stable <100>{100} loop. Calculation of the additional energy for conjunction of an original ½<111> loop and its transformation to a <100> segment is still not possible. However, if we assume this additional energy to be in the order of that of a double kink, i.e. ~0.5 eV. Then total barrier for gradual reorientation will be in the order of ~1.7 eV

Summarizing the above discussion:

The transformation barrier for the proposed mechanism is ~1.7 eV, corresponding to a transition temperature of 640 K, which is only slightly lower than the reported experimental value of 673 K.

Conclusions

A new mechanism of loop formation and transformation by self-interstitial atoms aggregation is proposed.
It shows how the change of Burgers vector of small loops from ½<111> to <100> in Fe-materials can possibly result from the re-arrangement and reorientation of crowdion clusters, without reactions with other dislocations.