EFDA
EUROPEAN FUSION DEVELOPMENT AGREEMENT

Structural Materials for Fusion Power Plants

Part III: Combining Experiments & Modelling for Effective Pathways to Develop New Structural Materials

Presented by J.-L. Boutard, EFDA-CSU Garching (Germany)

Phase Stability is Essential

What type of Modelling?

The Classical Thermodynamics Approach, which is Extremely Useful to Optimise Chemical Composition (see S. Zinkle)

and

Need for a Cohesive Model well-defined at the scale of the Chemical Bond & describing the various

Phase Stability and Phase Diagram: (1) Generalities

- **Phase stability of an alloy formed with atoms A and B**

  One crystal structure common to metals A &B:
- Alloy: **total of N atoms** with a **B concentration equal to c**

  Nc atoms A and N(1-c) atoms B
- Let Z be the co-ordinance number: number of First Nearest

  Z=8 for bcc, Z=12 for fcc
- At temperature T & pressure P, the stability of A_{1-c} B_c will be given by the minimum of the Gibbs free energy:

$$G=H-TS$$

Phase Stability and Phase Diagram: (2) Calculation of The Gibbs free energy

- **Enthalpy at 0 K: we assumed:**
  - it can be calculated on a **pair-wise assumption**:
    - H_{AA}, H_{AB}, H_{BB} are the pair enthalpies at 0K
  - The **random solid solution** formed by Nc B atoms & N(1-c) A atoms

$$H_0 = P_{AA}H_{AA} + P_{AB}H_{AB} + P_{BB}H_{BB}$$

$$P_{AA} = (1/2)N(1-c)Z(1-c) = (1/2)NZ(1-c)^2$$

$$P_{AB} = NcZ(1-c) = NZc(1-c)$$

$$P_{BB} = (1/2)NcZc = (1/2)Zc^2$$

$$H_0 = (1/2)ZN(1-c)H_{AA} + (1/2)ZNcH_{BB} + ZNc(1-c)\Omega$$

Enthalpy of a solid with N(1-c) atoms A

Enthalpy of a solid With Nc atoms B

Enthalpy of Mixing

Phase Stability and Phase Diagram: (2) Calculation of the Gibbs free energy (cont'd)

- Enthalpy of mixing at 0K: H_{mix} has the sign of Ω

$$H_{mix} = NZc(1-c)\Omega$$

with

$$\Omega = H_{AB} - (1/2)(H_{AA} + H_{BB})$$

Ω = 0 Ideal Solution

Ω > 0: Tendency to unmixing

Ω < 0: Tendency to Solid Solution

- Enthalpy at TK:

$$H = H_0 + \int_0^T C_p dT$$

- Vibration & Magnetic entropy:

$$S_{vibr} + S_{mag} = \int_0^T \frac{C_p}{T} dT$$

- Configuration entropy:

$$S_{Conf} = -k_B N[cLnc + (1-c)Ln(1-c)]$$

$$G = H_0 - TS_{Conf} + \int_0^T C_p dT - T\int_0^T \frac{C_p}{T} dT$$

Phase Stability and Phase Diagram: (3) Minimizing the Gibbs free energy

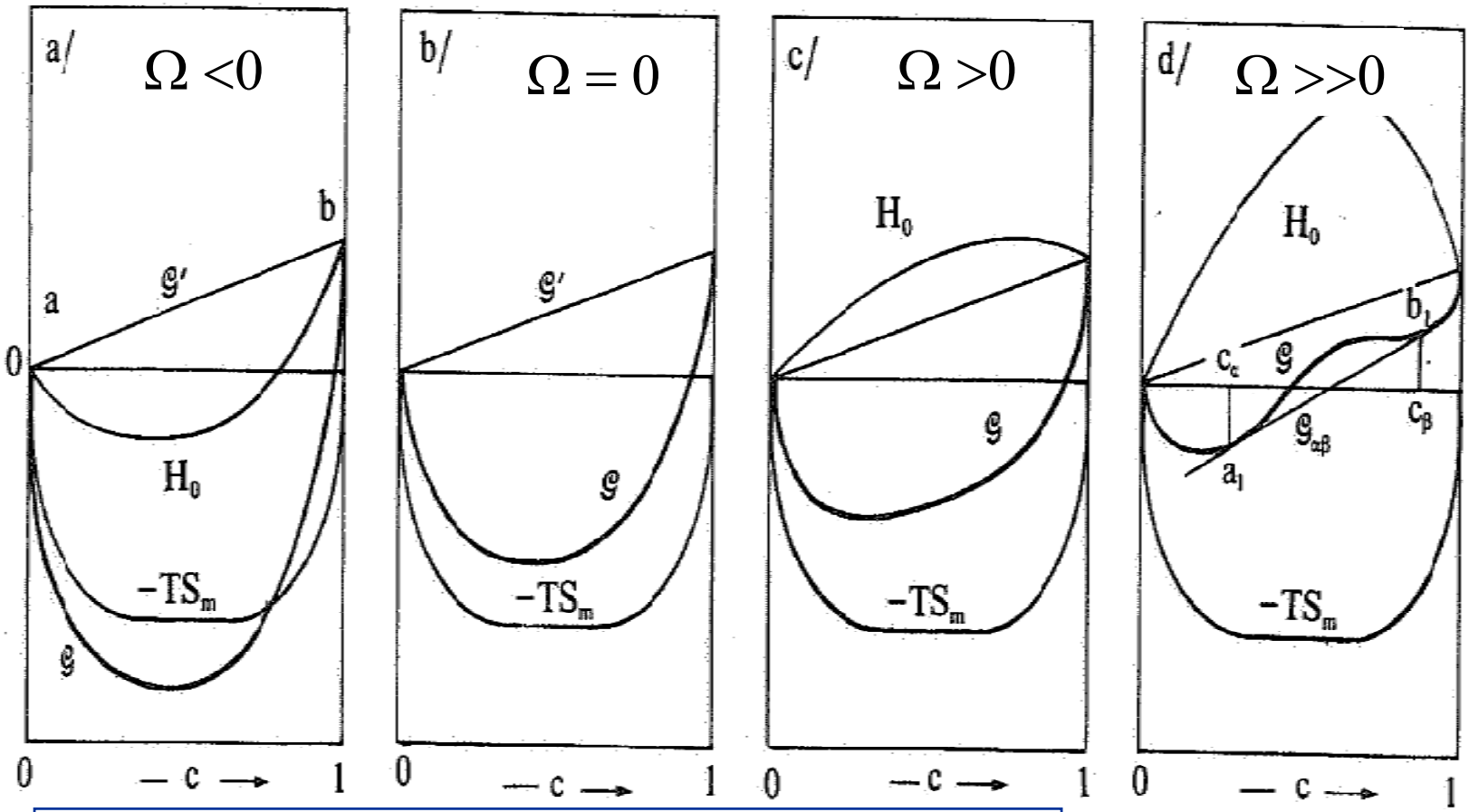
$$G = H_0 - TS_{Conf} + \int_0^T C_p dT - T\int_0^T \frac{C_p}{T} dT$$

The **second & third term** depending on the lattice vibration are **slowly depending on c**, especially if A & B are close in the Periodic table such as Fe and Cr, therefore one looks for the minimum of $\mathcal{G}$ versus the concentration c:

$$\mathcal{G} = H_0 - TS_{Conf}$$

Phase Stability versus Ω

$$\mathcal{G} = H_0 - TS_{Conf}$$



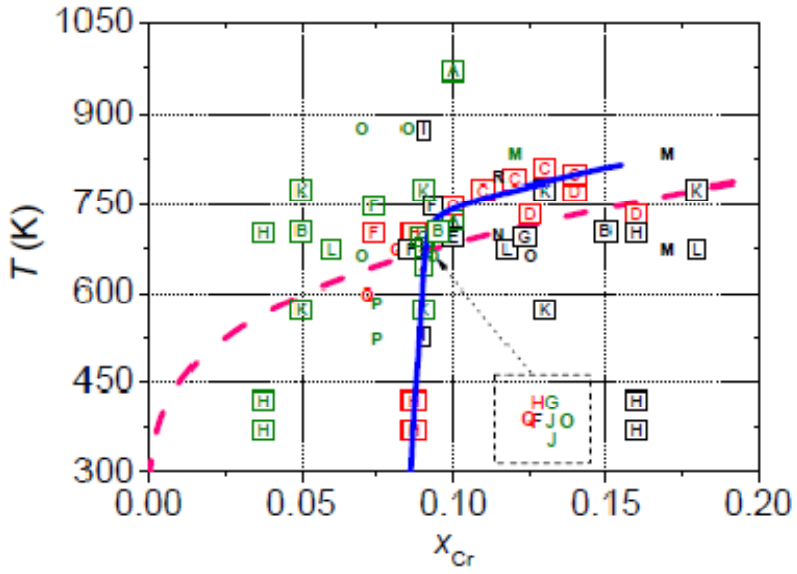
Complete Solid Solution

Miscibility Gap

CALPHAD Approach (1)

- **Gibbs Free Energy**

$$G_{tot}^{bcc} = cG_{Cr}^{bcc} + (1-c)G_{Fe}^{bcc} + G_{mix}^{bcc} + G_{Mag}^{bcc} + RT[cLnc + (1-c)Ln(1-c)]$$



Cr in solid solution in α-Fe

up to ~10 %Cr

- **Gibbs Free Energy of Mixing**

$$G_{mix}^{bcc} = (1-c)c\sum_{p=0}^{n} L_p^{bcc}(T)(2c)^p$$

- **Redlich-Kister Polynomials**

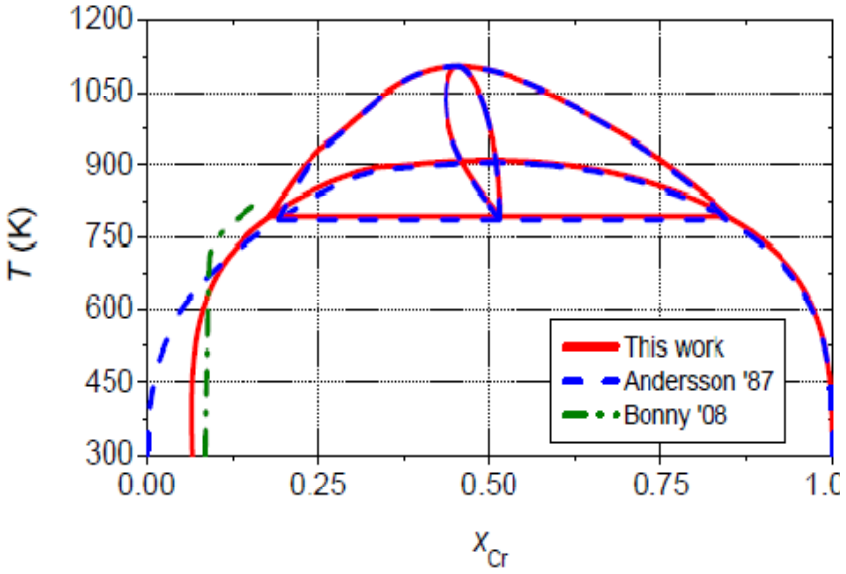
$$L_p^{bcc}(T) = l_0^p + l_1^p T + l_2^p T^2 + l_3^p T^3$$

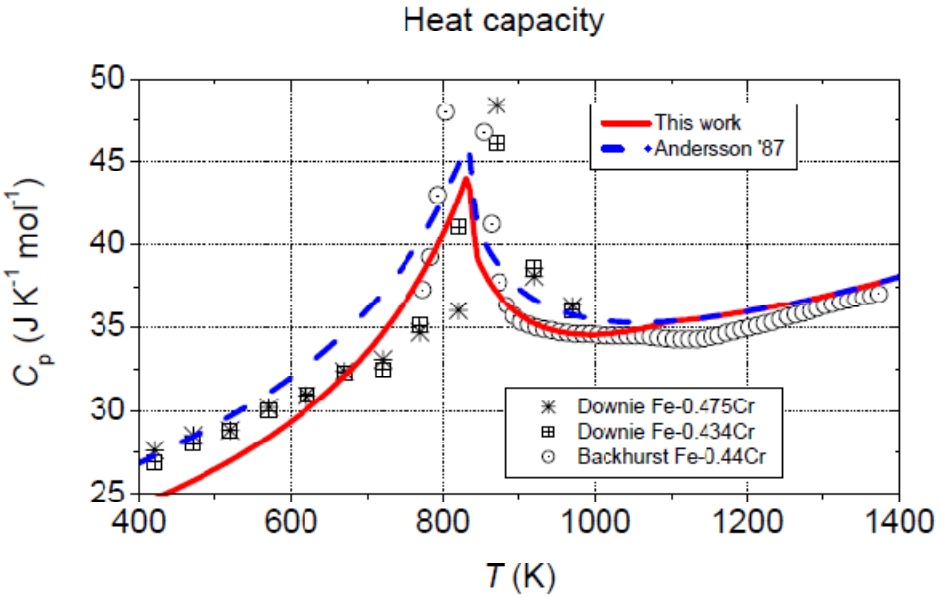
- G_{Mag}^{bcc}

Magnetic Gibbs Free Energy: by Integration of the Specific Heat data with an Empirical Form for the Magnetic Contribution [1].

[1] M. Hillert et al. CALPHAD 2, n0 3, 227-238.

CALPHAD Approach (2)





CLAPHAD **is based on Macroscopic Properties** treated in the **well established framework of Thermodynamics.**

CALPHAD is **not based on a Cohesive Model defined at the Scale of the Chemical bond** and **required for Multi-scale Modelling of Radiation Effects**

PHASE STABILITY MODELLING of Fe-Cr

based on a Physical description

of the Chemical Bond including Magnetism Explicitly

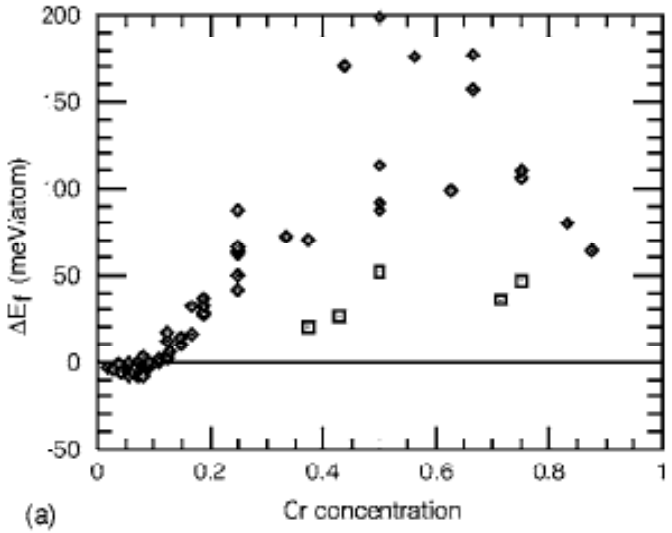
How to bridging the gap between Formation energies via DFT calculation at 0K and the Gibbs Free Energy ?

Activity 2 & 3: Need for Hamiltonian & Potentials (1)

Knowledge

DFT Calculation Formation Energy of

A Limited Number of Configurations at 0K



T.P.C. Klaver et al. PRB, 74, 094435 (2006)

Predictions

- **Phase Diagram: ⇔Free Gobbs Energy**

$$G = -k_B T.Ln[\sum_{n,V} g_n \exp(-\frac{E_n + p_0 V}{k_B T})]$$

Mean Field Theory of Transport controlled by Diffusion:

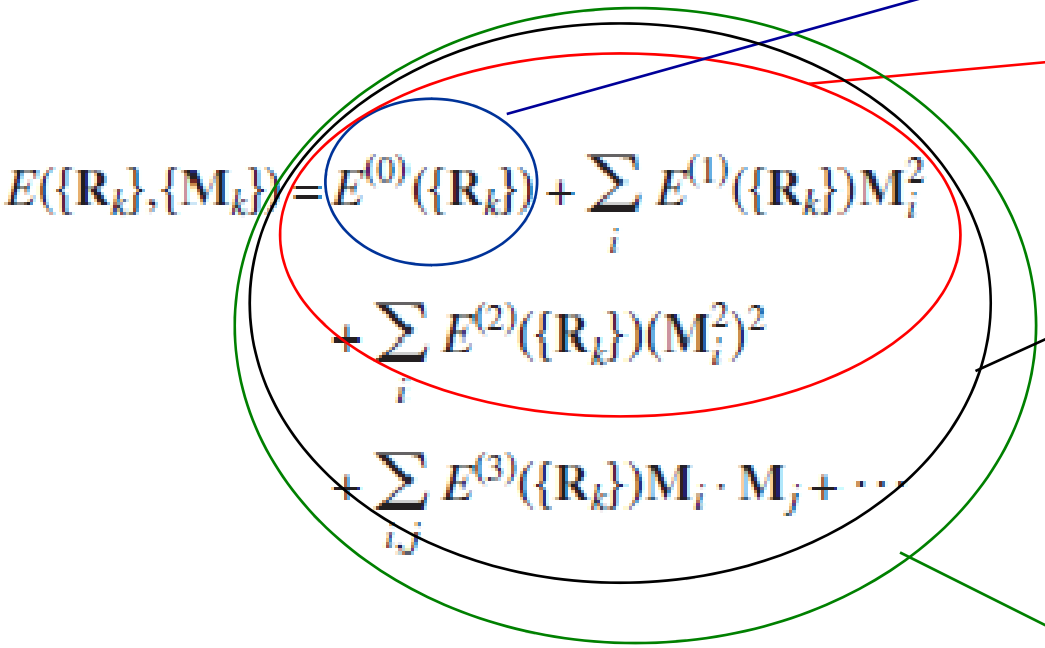
$$J_i = -\sum_j L_{i,j} \nabla \mu_j \qquad \mu_j = (\frac{\partial G}{\partial x_j})_{T,P,x_{i \neq j}}$$

Molecular Dynamics: forces are the derivatives of the potential.
The whole energy spectrum with configuration, lattice and magnetic excitations is **required.**

Potentials/Hamiltonians are to be developed
From a limited number of Configurations
to describe the Complete Energy Spectrum of the Fe-Cr System

Activity 2 & 3: Need for Hamiltonian & Potentials (2)

- The requested Hamiltonian has the general form satisfying invariance rules [1]



- **Two-band EAM potential**
- Magnetic Potential
- **Magnetic Cluster Expansion (MCE): $R_k=R_{ok}$=Constant Configuration & Magnons Entropy**
- **"High T" Hamiltonian Configuration, Phonons, Magnons Entropy (> 2009)**

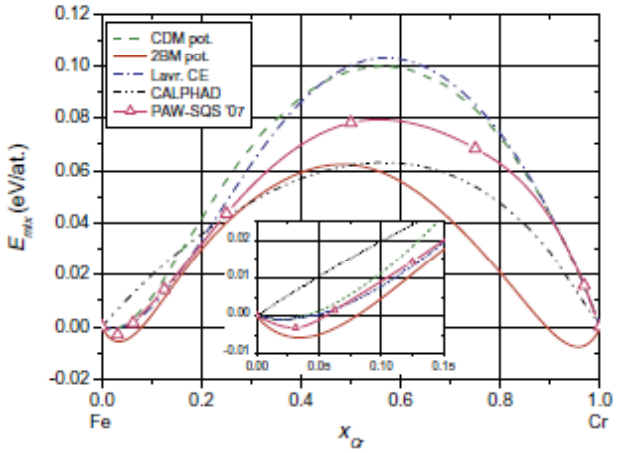
[1] Pui-Wa Ma, C.H. Woo, S.L. Dudarev PRB 78, 024434 (2008)

Two-band Potential

- **Two band Potential: EAM potential with two embedded terms, one for the d-bands & another one associated with s-band**

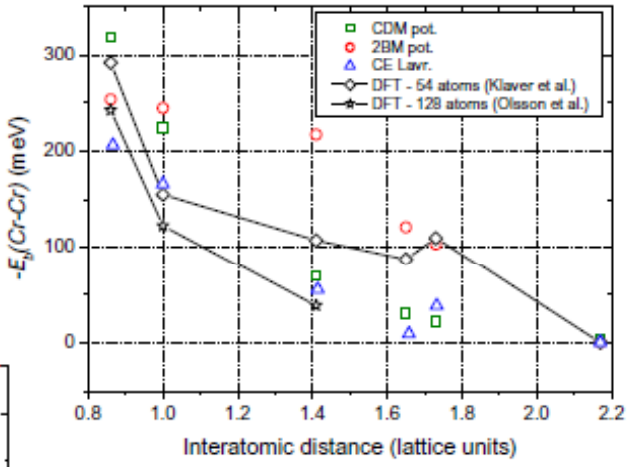
In the Fe-rich domain of the Fe-Cr System

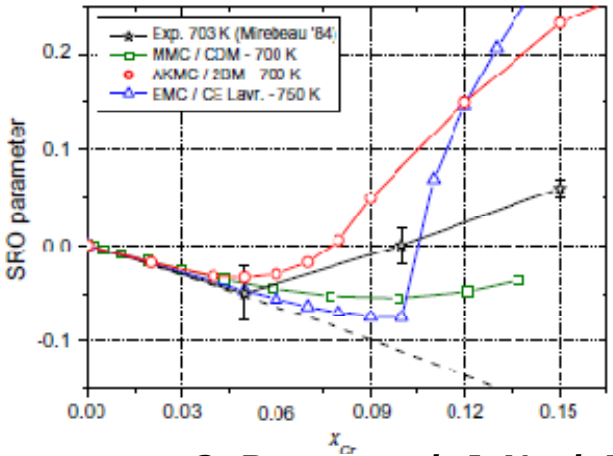
Present 2-band potential reproduces quite well:



Negative Enthalpy of mixing

Repulsive Energy between Cr atoms





Short Range Order of Cr atoms

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CENTRE D'ÉTUDE DE L'ÉNERGIE NUCLÉAIRE

G. Bonny et al. J. Nucl. Mater. (2009) In Press

PHASE STABLITY MODELLING of Fe-Cr

How to treat Ferro-magnetism with Realistic Physical Assumption?

Hamiltonian for 3 d Magnetic metals: (1) Tight Binding Approximation

$$H = \sum_{i,m,\sigma} \varepsilon_i n_{im\sigma} + \sum_{i,j,i\neq j} \sum_{m,m',\sigma} t_{im,jm'} n_{im\sigma} n_{jm'\sigma} + \sum_i H_i$$

Chemical Bond:

One site Energy ε_i + Hopping term $t_{i,m,j,m'}$

On-site Interaction

$$H_i = \overline{U} \sum_{m,m'} n_{i,m,\uparrow} n_{i,m',\downarrow} + \frac{\overline{U} - \overline{J}}{2} \sum_{m\neq m'} (n_{i,m,\uparrow} n_{i,m',\uparrow} + n_{i,m,\downarrow} n_{i,m'\downarrow})$$

U ~10 eV: Effective Energy of interaction between two electrons with Anti-parallel Spin

J~1eV: Intra-atomic Exchange Energy GAIN when two electrons with Same Spin are in two Different Orbitals

S. L. Dudarev and P. M. Derlet Proceeding of the MMM-3 Freiburg (G) 18-22, pp 713-720

Hamiltonian for 3 d Magnetic metals: (2) Stoner Term

$$H_i = \overline{U} \sum_{m,m'} n_{i,m,\uparrow} n_{i,m',\downarrow} + \frac{\overline{U} - \overline{J}}{2} \sum_{m \neq m'} (n_{i,m,\uparrow} n_{i,m',\uparrow} + n_{i,m,\downarrow} n_{i,m'\downarrow})$$

Introducing the number of electrons

with spin up $N_\downarrow$ & Spin down $N_\uparrow$

$$H_i = \overline{U} N_\uparrow N_\downarrow + \frac{\overline{U} - \overline{J}}{2} [N_\uparrow (N_\uparrow - 1) + N_\downarrow (N_\downarrow - 1)]$$

Introducing the total number of electrons $N = N_\uparrow + N_\downarrow$

and the magnetic moment $\zeta = N_\uparrow - N_\downarrow$

$$H_i = \frac{\overline{U}}{2} N(N-1) - \frac{\overline{J}}{2} N(N+2) - \frac{\overline{J}}{4} \zeta^2 \approx \frac{\overline{U}}{2} N(N-1) - \frac{\overline{J}}{4} \zeta^2$$

Coulomb on-site repulsion: Could prevent hopping Metal → Mott insulators

Only one Magnetic term, the Stoner term proportional to the exchange interaction

S. L. Dudarev and P. M. Derlet Proceeding of the MMM-3 Freiburg (G) 18-22, pp 713-720

Hamiltonian for 3 d Magnetic metals: (3) Ferro-magnetism vs Para-magnetism Stability

$$E_{tot}(N,\zeta) = \int_{-\infty}^{\varepsilon_{F\uparrow}} E.D(E).dE + \int_{-\infty}^{\varepsilon_{F\downarrow}} E.D(E).dE - \bar{J}.\zeta^2/4 \qquad \textbf{(1)}$$

$$N = \int_{-\infty}^{\varepsilon_{F\uparrow}} D(E).dE + \int_{-\infty}^{\varepsilon_{F\downarrow}} D(E).dE = cst. \qquad \textbf{(2)}$$

$$\zeta = \int_{-\infty}^{\varepsilon_{F\uparrow}} D(E).dE - \int_{-\infty}^{\varepsilon_{F\downarrow}} D(E).dE = \int_{\varepsilon_{F\downarrow}}^{\varepsilon_{F\uparrow}} D(E).dE \qquad \textbf{(3)}$$

The Equilibrium Magnetic moment is obtained by solving the equations obtained by :

- writing that the total energy is an Extremum and
- derivating versus ζ the equations giving
  (i) the total number of electrons (ii) the magnetic moment

$$\varepsilon_{F\uparrow} D(\varepsilon_{F\uparrow}) \frac{\partial \varepsilon_{F\uparrow}}{\partial \zeta} + \varepsilon_{F\downarrow} D(\varepsilon_{F\downarrow}) \frac{\partial \varepsilon_{F\downarrow}}{\partial \zeta} - \frac{1}{2}\bar{J}\zeta = 0 \qquad \textbf{(4)}$$

$$D(\varepsilon_{F\uparrow}) \frac{\partial \varepsilon_{F\uparrow}}{\partial \zeta} + D(\varepsilon_{F\downarrow}) \frac{\partial \varepsilon_{F\downarrow}}{\partial \zeta} = 0 \qquad \textbf{(5)}$$

$$D(\varepsilon_{F\uparrow}) \frac{\partial \varepsilon_{F\uparrow}}{\partial \zeta} - D(\varepsilon_{F\downarrow}) \frac{\partial \varepsilon_{F\downarrow}}{\partial \zeta} = 1 \qquad \textbf{(6)}$$

S. L. Dudarev and P. Derlet, J Phys.:Cond. Matter 17 (2005) 7097-7118

Hamiltonian for 3 d Magnetic metals: (4) Ferro-magnetism vs Para-magnetism Stability

- The Equilibrium momentum is given by

$$\zeta_0 = \frac{\varepsilon_{F\uparrow}(N,\zeta_0) - \varepsilon_{F\downarrow}(N,\zeta_0)}{\overline{J}}$$

$\varepsilon_{F\uparrow}(N,\zeta_0)$ & $\varepsilon_{F\downarrow}(N,\zeta_0)$ being given by:

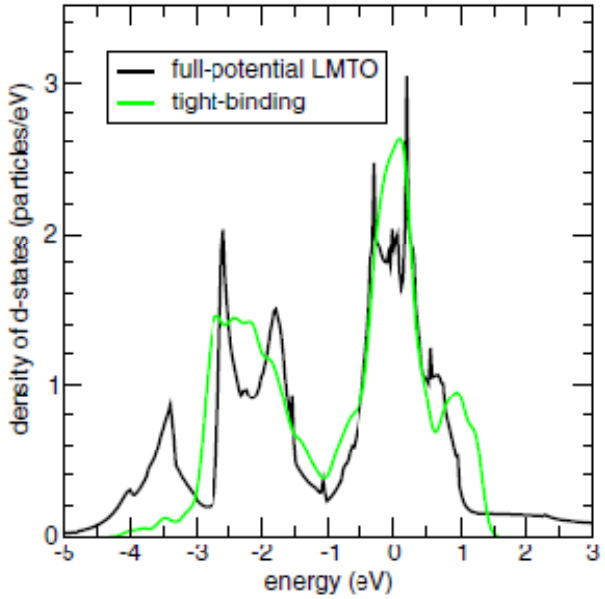
$$\overline{J}\,\frac{\int_{\varepsilon_{F\downarrow}}^{\varepsilon_{F\uparrow}} D(E)dE}{[\varepsilon_{F\uparrow}(N,\zeta_0) - \varepsilon_{F\downarrow}(N,\zeta_0)]} = 1$$

- The stability condition is: Energy is minimum at ζ_0: $\frac{d^2E(N,\zeta)}{d\zeta^2} > 0$

$$\frac{1}{2}\left[\frac{1}{D(\varepsilon_{F\uparrow})} + \frac{1}{D(\varepsilon_{F\downarrow})}\right] - \overline{J} > 0$$

S. L. Dudarev and P. Derlet, J Phys.:Cond. Matter 17 (2005) 7097-7118

Hamiltonian for 3 d Magnetic metals: (5-a) Form of the Magnetic Energy



Using the Density of State Calculated ab initio or within tight binding approximation

Equations (1), (2) and (3) are solved numerically

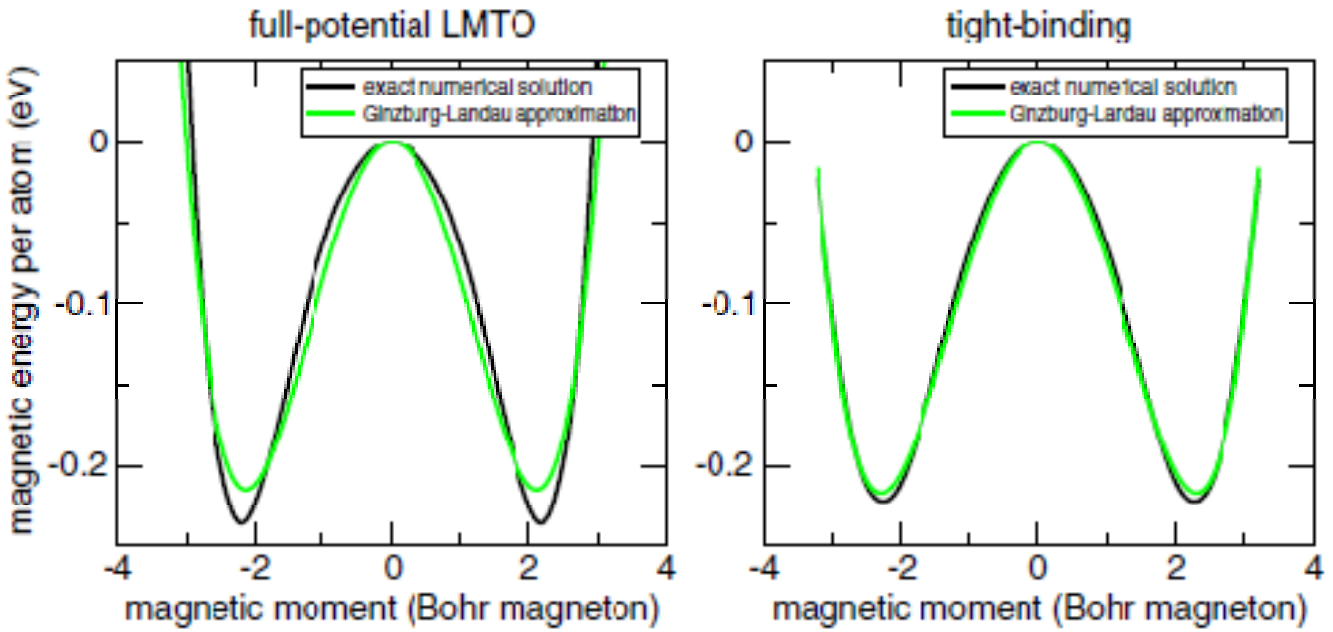
$$E_{tot}(N,\zeta) = \int_{-\infty}^{\varepsilon_{F\uparrow}} E.D(E).dE + \int_{-\infty}^{\varepsilon_{F\downarrow}} E.D(E).dE - \overline{J}.\zeta^2/4 \qquad (1)$$

$$N = \int_{-\infty}^{\varepsilon_{F\uparrow}} D(E).dE + \int_{-\infty}^{\varepsilon_{F\downarrow}} D(E).dE = cst. \qquad (2)$$

$$\zeta = \int_{-\infty}^{\varepsilon_{F\uparrow}} D(E).dE - \int_{-\infty}^{\varepsilon_{F\downarrow}} D(E).dE = \int_{\varepsilon_{F\downarrow}}^{\varepsilon_{F\uparrow}} D(E).dE \qquad (3)$$

S. L. Dudarev and P. Derlet, J Phys.:Cond. Matter 17 (2005) 7097-7118

Hamiltonian for 3 d Magnetic metals: (5-b) Form of the Magnetic Energy



$$E_{tot}(N,\zeta) - E(N,0) = \alpha\zeta^2 + \beta\zeta^4$$

The simplest model of a second-order phase transition: the Ginzburg-Landau Model applies

α =-8.22x10-2 eV, β=7.78x10-3 eV and $\zeta_0 = (-\alpha/2\beta)^{1/2}$ =2.26 μ_B

S. L. Dudarev and P. Derlet, J Phys.:Cond. Matter 17 (2005) 7097-7118

The Magnetic Cluster Expansion of Fe-Cr

Magnetic Cluster Expansion

$$H(\{\sigma\},\{M\}) = NJ^{(0)} + \sum_i J_i^{(1)}\sigma_i + \sum_{i,j=NN} J_{ij}^{NN}\sigma_i\sigma_j + \sum_{i,j=NNN} J_{ij}^{NNN}\sigma_i\sigma_j$$

$$\sum_i (A^{(0)} + A^{(1)}\sigma_i + \sum_{j=NN} A^{NN}\sigma_i\sigma_j + \sum_{j=NNN} A^{NNN}\sigma_i\sigma_j)\mathrm{M}_\mathrm{i}^2$$

$$\sum_i (B^{(0)} + B^{(1)}\sigma_i + \sum_{j=NN} B^{NN}\sigma_i\sigma_j + \sum_{j=NNN} B^{NNN}\sigma_i\sigma_j)\mathrm{M}_\mathrm{i}^4$$

$$-\sum_i \sum_{j=NN} [I_{NN}^{(0)} + I_{NN}^{(1)}(\sigma_i + \sigma_j) + I_{NN}^{(1)}\sigma_i\sigma_j]\mathrm{M}_\mathrm{i}\mathrm{M}_\mathrm{j}$$

$$-\sum_i \sum_{j=NNN} [I_{NNN}^{(0)} + I_{NNN}^{(1)}(\sigma_i + \sigma_j) + I_{NNN}^{(1)}\sigma_i\sigma_j]\mathrm{M}_\mathrm{i}\mathrm{M}_\mathrm{j}$$

$$-\ldots.$$

σ_i=+1 Fe on site i

σ_j=-1 Cr on site j

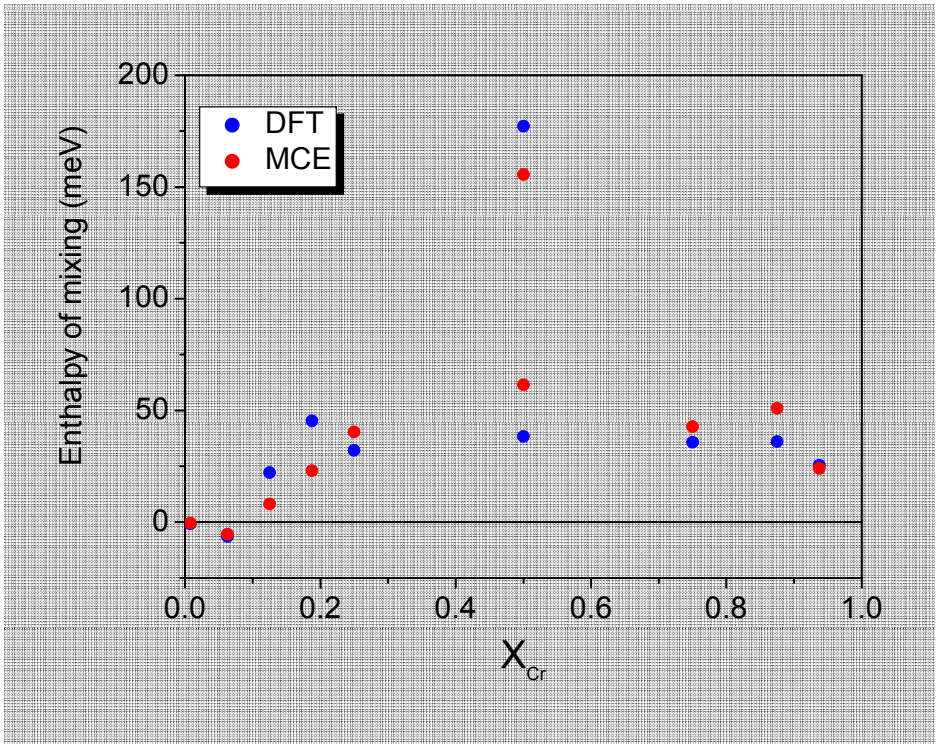
Pair interactions

- **Fitted on DFT Enthalpies of mixing & A, B, I, J, M_i, M_j** $\partial H / \partial M_i = 0$

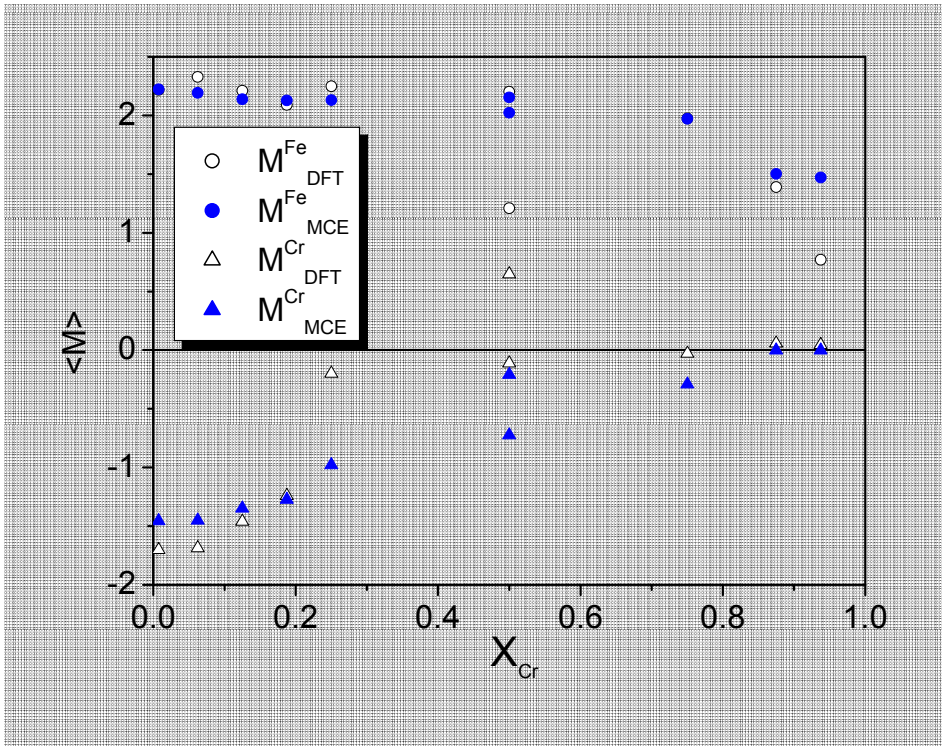
Magnetic Cluster Expansion

MCE fitted on DFT Enthalpy of Mixing allows reproducing:

DFT Enthalpy of Mixing



DFT Magnetic Moment



Monte Carlo Simulation of

Magnetic Properties, Specific heat & Free Energy have been carried out

Specific Heat of pure α-Fe

Cluster Magnetic Expansion

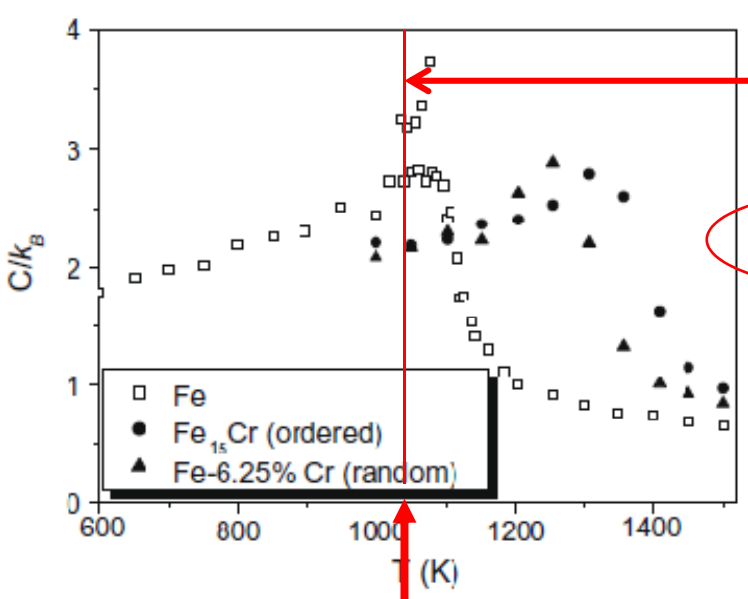
M. Yu. Lavrentiev et al J. Nucl. Mater, (2009) in press

$$C_{Mag} = \frac{< E^2 > - < E >^2}{k_B T^2}$$

CALPHAD

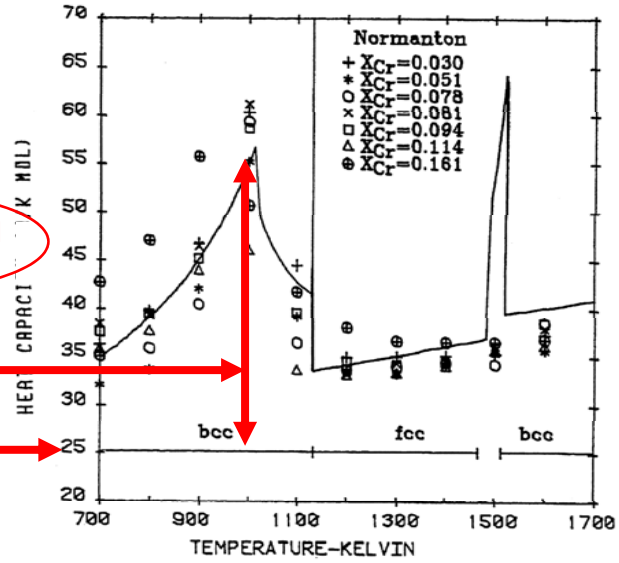
J-O Andersson & B. Sundman, Calphad 11 (1987) 83-92

$$C_p = -T \frac{\partial^2 G}{\partial T^2}$$



~30 JK^{-1}mol^{-1}

3R



T_{Curie} (α-Fe) =1050 K

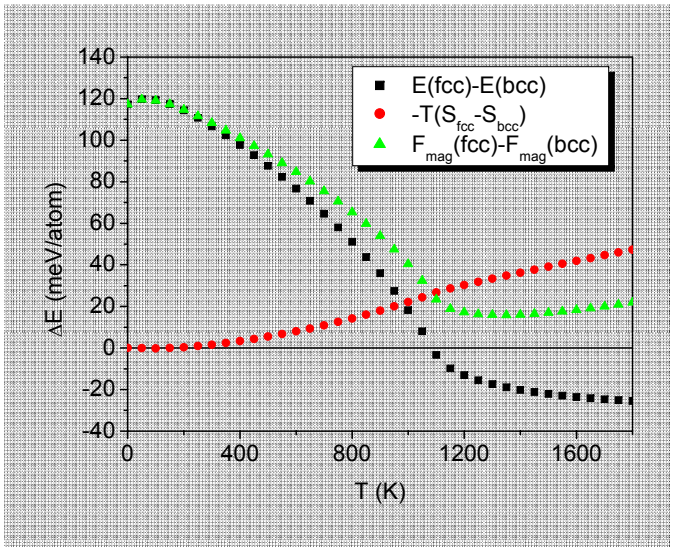
Excellent Prediction of the Magnetic Cluster Expansion

Magnetic Cluster Dynamics

Monte Carlo Simulation of the Free Energy:

Configuration Entropy

Magnetic Excitation Entropy



Not sufficient to Stabilise the fcc (γ) at High Temperature

Adding

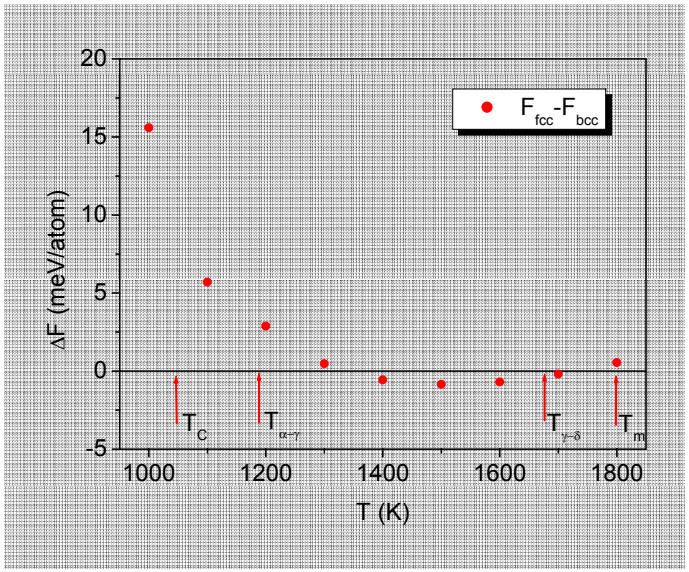
Phonons entropy based on experimental data (Neutron Diffraction & Elastic Constants

Monte Carlo Simulation of the Free Energy:

Configuration Entropy

Magnetic Excitation Entropy

Experimental Phonons entropy



For the *First Time* the high T "γ loop" of iron is predicted based on DFT and atomistic modelling & experimental data

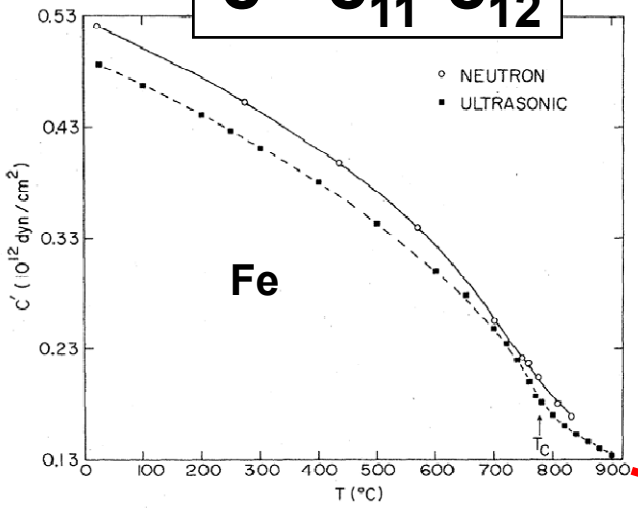
Physically based Modelling Plasticity

- **Low Temperature (see PartII)**
  - Mobility of Screw Dislocation
  - Peierls Barrier
  - Double kink formation enthalpy

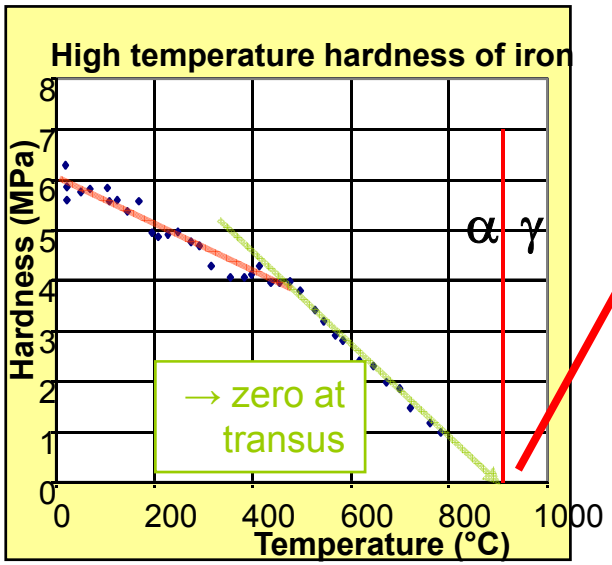
- **High temperature Softening of α-Fe and bcc Steels**
  - Stability of <100> Burgers vector dislocation versus ½<111>
  - Prediction of elastic constant
  - Anisotropic Elasticity for α-Fe and bcc steels

Anisotropic Elasticity, Hardness, Phase Diagram

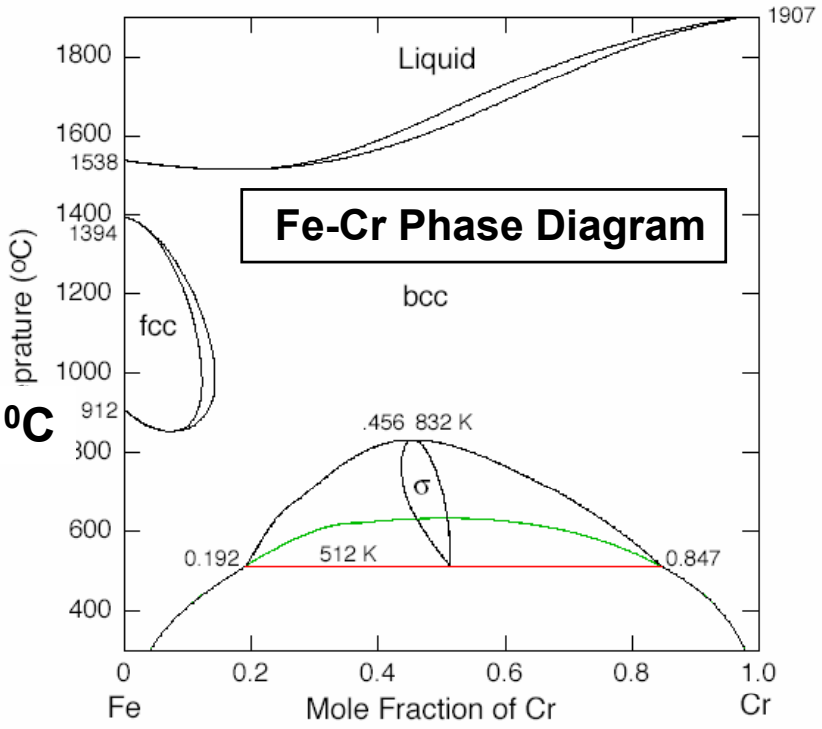
$c' = c_{11} - c_{12}$



912 ^{0}C

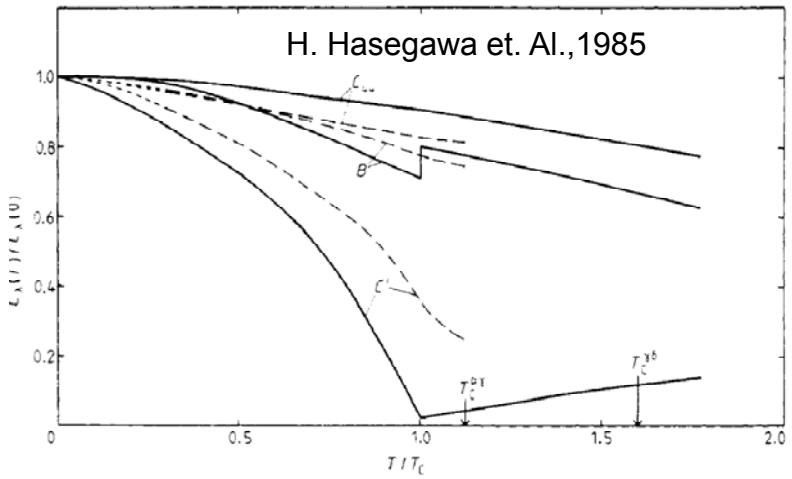


J.H. Westbrook, *Rev. Hautes Temper. & Refrac.*, **3** (1966), 47.



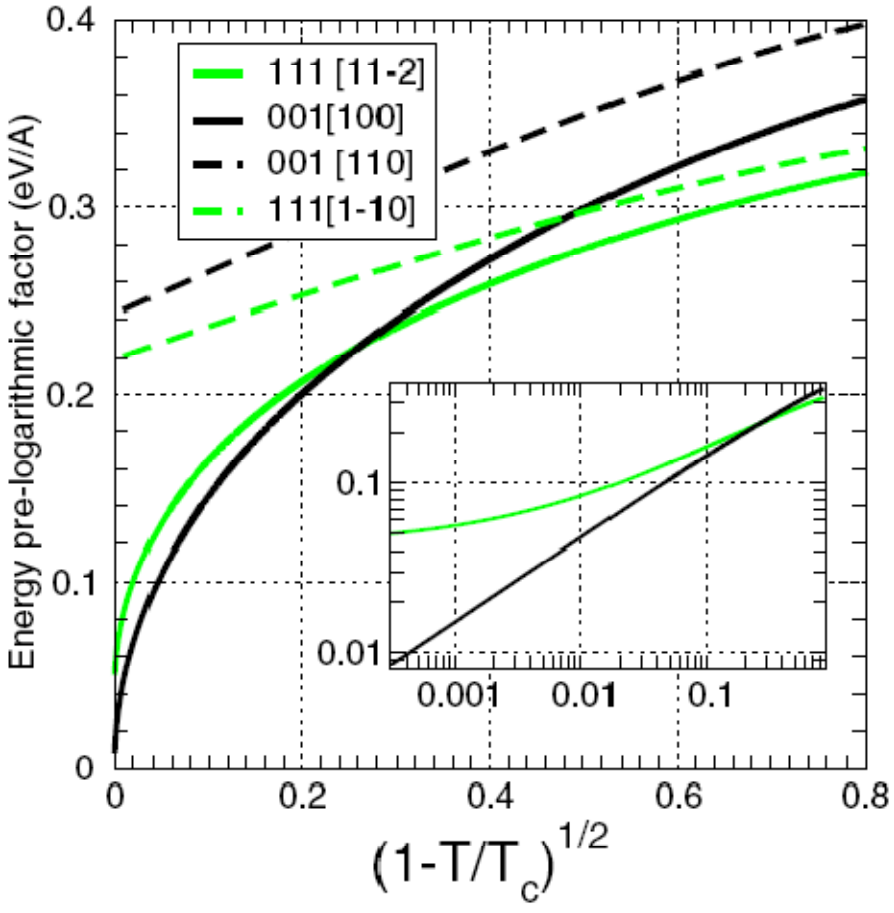
Tetragonal Shear elastic constant and Hardness of α-Fe decrease gradually with temperature in a fully consistent way with phase diagram

<111> dislocations in α-Fe: the α-γ magnetic instability



Thermal spin fluctuations in iron : One of the elastic constants $c'=c_{11}-c_{12}$ nearly vanishes near the α-γ phase transition point (912 ^{0}C).

$$K_{001}([100]) = \frac{a^2}{4\pi}(c_{11}+c_{12})\left[\frac{c_{44}(c_{11}-c_{12})}{c_{11}(c_{11}+c_{12}+2c_{44})}\right]^{1/2}$$

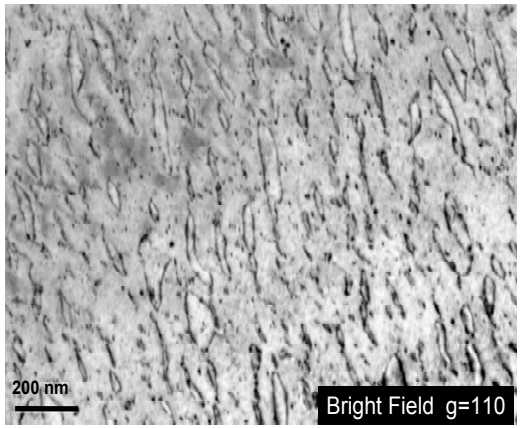


The *anisotropic* elastic *free* self-energy of <100> dislocations vanishes near the α-γ phase transition temperature, driving the <111> to <100> Burgers vector transformations.

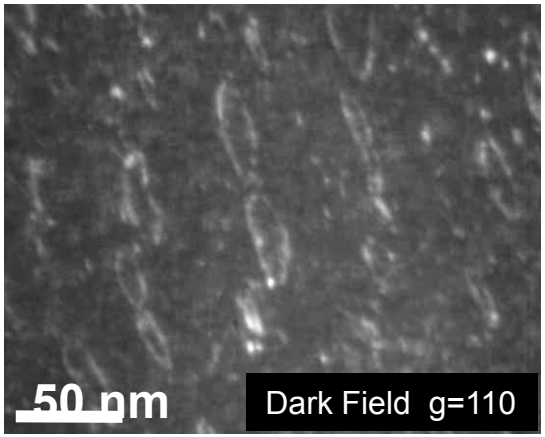
PRL S. Dudarev, R. Bullough and P.Derlet 100 (2008) 135503.

<111> dislocations in α-Fe: the α-γ magnetic instability

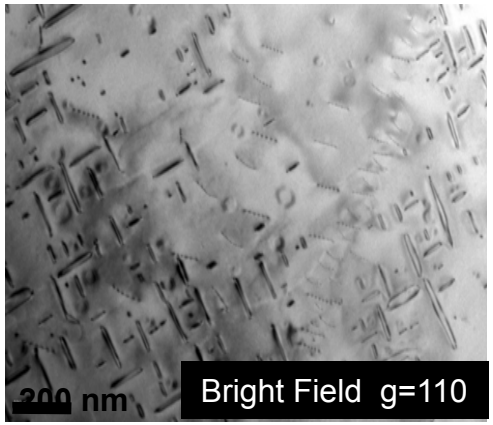
Predominantly a/2<111>Bürgers vectors



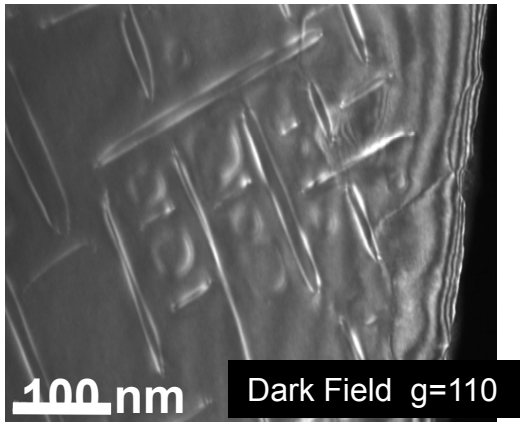
UHP-Fe irradiated at 300°C
Dose: 1x10^{19} ions m^{-2}



Predominantly a<100>Bürgers vectors



UHP-Fe irradiated at 500°C
Dose: 1x10^{19} ions m^{-2}



UKAEA Fusion Working in Europe

EPSRC

Zhongwen Yao, John Murphy, Mike Jenkins & Sergei Dudarev, Dislocations 2008

High Temperature Softening of bcc Steels

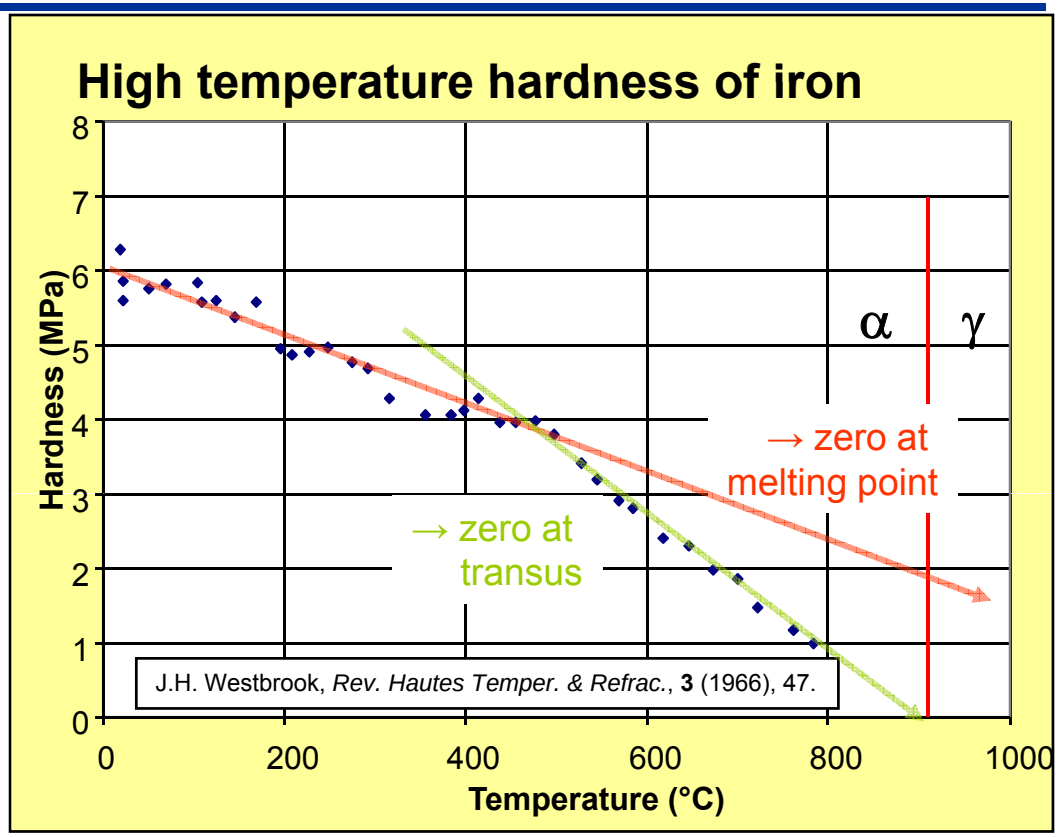
A/r

1. Repulsive force between two similar dislocations.

(r is their separation. A depends on the elastic constant)

2. "A" governs Pile-up resistance to shear & Yield of the materials

$$A_{\langle 100\rangle[001]} \approx \frac{1}{4\pi}\sqrt{\frac{C' C_{12} C_{44}}{C_{12} + C_{44}}},$$



- **Hardness falls towards zero at the α – γ transus temperature (910°C).**

Shear instability of the bcc-α structure with respect to the fcc -γ structure at the transus.

- **Change of slope of the hardness curve at about 500°C.**

Tentatively identified with this with the change in active dislocation above ~500°C

Zhongwen Yao, John Murphy, Mike Jenkins & Sergei Dudarev, Dislocations 2008

Strategic Objectives 2010-2015

Fusion Materials Topical Group, March 2009 EFDA-D-2D4B78

STRATEGIC OBJECTIVES FOR FUSION MATERIALS MODELLING AND EXPERIMENTAL VALIDATION (2010-2015).

J.-L. Boutard [1], M.J. Caturla [2], S.L. Dudarev [3], F. Willaime [4]

[1] *EFDA Close Support Unit, Garching, Germany*
[2] *Universidad de Alicante, Departamento de Fisica Applicada, Spain*
[3] *EURATOM/UKAEA Fusion Association, Culham, UK*
[4] *CEA/Saclay, Service de Recherche de Métallurgie Physique, France.*

Executive summary

This document gives a summary of key recent results achieved by the EFDA materials modelling and experimental validation programme, and outlines specific future objectives that, if achieved, will bring the programme to the goal of having available a comprehensive yet conceptually transparent predictive model for EUROFER-type steels.

The breakdown of objectives given in the document goes beyond stating general needs, and highlights the key physical phenomena, the development of mathematical description and experimental validation for which should advance the program to a level where computer modelling becomes capable of driving innovative development of promising candidate fusion materials.

Acknowledgements: E. Diegele, P.M. Derlet, K. Nordlund, L. Malerba, S.G. Roberts, D. Terentyev

http://www.efda.org/eu_fusion_programme/scientific_and_technical_publications.htm

Reasons for success of the current/future effort:

- ***New ideas*** for solving problems: expertise and scientific & technical competence.
- ***Integrated approach*****,** with objectives remaining constant over reasonably extended periods of time.
- **EUROFER to remain the central objective**, with spin-offs expected for other materials, as before (tungsten, ODS, other alloys). Work will focus on (see detailed breakdown in "STRATEGIC OBJECTIVES"):
  1. **Cohesion, including high temperature effects,**
  2. **Phase stability under irradiation and phase diagrams,**
  3. **Atomistic dynamics of radiation damage,**
  4. **Helium, hydrogen and damage accumulation,**
  5. **Plasticity and fracture,**
  6. **Visco-plasticity and creep**.
- **Method: closely linked modelling and experimental validation** studies.
- **Collaboration between laboratories/individual groups** involved, **regular monitoring twice a year with common assessment & definition of objectives to be addressed via Calls for Propsoals.**

Highlights (I):

- Assess, **by the 0K *ab-initio* calculations**, **the structures formed by the main chemical constituents of (unirradiated) EUROFER steel**. Create an accessible and verified database of crystal structures for Fe-Cr model alloys, **α and α' phases on body-centred cubic (bcc) and face-centred cubic (fcc) lattices**, as well as the representative structures for Fe-Cr-C, Fe-Cr-N, Fe-Cr-W, Fe-Cr-V, Fe-Cr-Ta, Fe-Cr-O cluster configurations, and ordered phases, related to the **formation of carbides, martensitic phases, and the σ-phase.**

- Develop **a Monte Carlo model**, **explicitly including magnetism**, to quantitatively describe **the full Temperature-Concentration Phase diagram of the Fe-Cr system**, predicting the ***miscibility gap, the σ-phase and the γ-loop***.

- **Assess the effect of radiation defects on the phase stability of Fe-Cr alloys.** Develop a Monte-Carlo treatment for the phase nucleation events, and model growth of α' and σ phase precipitates under irradiation **(ballistic effects & point defects).** Determine how the finite temperature (free energy) effects associated with defects and dislocation cores influence nucleation of new ordered phases (for example α and σ-phases) under irradiation.

- Develop a model based on **Monte Carlo or Mean Field** approach of **diffusion mass transport** in **concentrated Fe-Cr-C alloys under irradiation**

Highlights (II):

- Develop ***a quantitative model for migration of He and hydrogen near surfaces & Grain-Boundaries in iron, Fe-Cr alloys, and tungsten***. Describe the observed ion implantation profiles, defect accumulation profiles, and the evolution of these profiles as a function of temperature, time, and irradiation dose rate. **Explain the combined synergetic effects of triple beam ion irradiation on swelling of Ferritic-martensitic steels.**

- Develop a **model for brittle fracture** of pure iron, and extend it to other bcc metals, including Fe-Cr alloys. Develop a model for **brittle fracture of *irradiated* iron**, other bcc metals, and Fe-Cr alloys. Explain the DBTT saturation effect observed in the limit of low helium transmutation rate. Assess the potential of high temperature operation for minimizing the radiation embrittlement effect. Explain why DBTT recovers if irradiation is performed at elevated temperatures close to or above 400°C in the absence of He production.

- Develop **Discrete Dislocation Dynamics (DDD) within the anisotropic elasticity theory of dislocations for α-Fe and Fe-Cr alloys.**

- **Couple DDD model with kinetic Monte Carlo or Mean field theory** describing diffusion of point defects **to describe dislocation climb under radiation and thermal creep conditions**

Summary:

Ambitious programme, which:

- will require **considerable effort for implementation & monitoring**
- is **focused on realistic, and necessary objectives.**
- benefits from having a **general framework and detailed objectives defined in the form of a reasonably well defined roadmap ("STRATEGIC OBJECTIVES").**

The new objectives are:

- **based upon existing developments that have already proven to be successful.**
- **fully consistent with the current and future needs of fusion technology** that require full qualification of existing, **and development of new blanket and plasma facing materials.**

What kind of Validation Experiments ? (1)

Modelling Oriented Experiments

- At the relevant scale
- On adequate systems
- With Rapid Feedback

Ion-beam Irradiation

in Single & Multiple Beam configuration

- Reliable and Versatile technique
- Volume irradiated/implanted compatible with all modern physical chemical characterization techniques
- With Rapid Feedback

Dual & Triple Beam Accelerator

Laboratory	Facilities	Application field	Reference
a) dual or triple MeV ion beams			
MSD, IGCAR Kalpakkam, India	1.7 MV Tandetron Ion implanter (30–150 keV)	Irradiation behaviour of nuclear alloys	[6]
HIT Tokyo, Japan	3.75 MV Van de Graaff 1 MV Tandetron	Irradiation behaviour of nuclear alloys and ceramics	[7]
DNE Nagoya University, Japan	2 MV Van de Graaff 200 kV ion implanter	Irradiation behaviour of nuclear alloys and ceramics	[8]
FZ Rossendorf, Germany	3 MV Tandetron 500 kV ion implanter	Synthesis of nanostructured ceramics assisted by irradiation Ion beam modification of materials	[9]
FSU Iena, Germany	3 MV Tandetron JULIA 400 kV ion implanter ROMEO	Synthesis of nanostructured ceramics assisted by irradiation Irradiation behaviour of nuclear alloys	[10]
IAE Kyoto, Japan	1.7 MV Tandetron 1 MV Van de Graaff 1 MV Singletron	Evolution of microstructure under multi-irradiation	[11]
JAERI Takasaki, Japan	3 MV Tandem 3 MV Van de Graaff 400 kV ion implanter	Synthesis of nanostructured ceramics assisted by irradiation Behaviour of alloys and ceramics under irradiation	[12]
DMN Saclay, France (ready to operate at the beginning of 2008)	3 MV Pelletron ÉPIMÉTHÉE 2.5 MV Van de Graaff YVETTE 2.25 MV Tandetron	Irradiation behaviour of nuclear materials Ion beam modification of materials	[13]

Y. Serruys et al., JANNUS: experimental validation at the scale of the atomic modelling, C. R. Physique (2007), doi:10.1016/j.crhy.2007.10.015

Single & Dual Beam Coupled toTEM

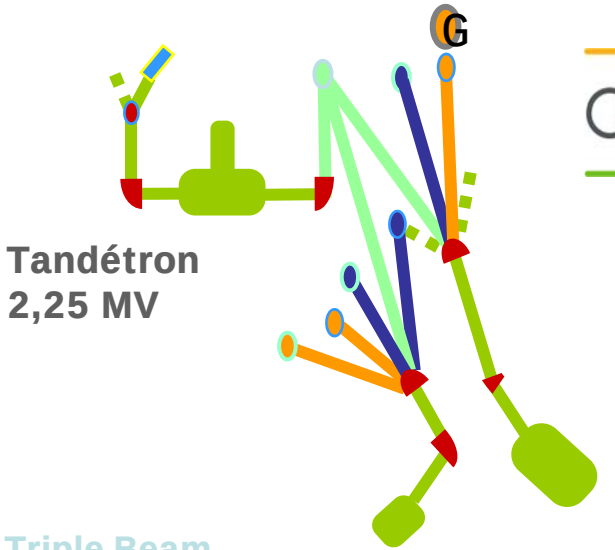
b) mono or dual ion beams (>100 keV) coupled to a TEM			
CARET Sapporo, Japan	1.3 MV HVTEM 400 kV ion implanter 300 kV ion implanter	Synthesis of nano-structured materials assisted by irradiation Behaviour of nuclear materials under irradiation	[14]
Argonne National Laboratory, USA	2 MV Tandem or 650 kV ion implanter 300 kV TEM	Irradiation behaviour of nuclear ceramics	[15]
CSNSM Orsay, France (ready to operate at the beginning of 2008)	2 MV Tandem/Van de Graaff ARAMIS 150 kV ion implanter IRMA 200 kV TEM	Irradiation behaviour of nuclear ceramics and semiconductors Ion beam modification of materials	[13]
c) dual keV ion beams coupled to a TEM			
IMR, University of Salford, UK (under construction)	200 kV TEM Ion implanter (5–100 keV, $A \leqslant 140$)	Radiation damage on nuclear reactor materials and semiconductors	[16]
JAERI DMD Takasaki, Japan	400 kV TEM 400 kV ion implanter 40 kV ion gun	Radiation effects	[17]
JAERI DMSE Tokai-Mura, Japan	2 × 40 kV ion guns 400 kV TEM	Irradiation behaviour of nuclear alloys and ceramics	[18]

Y. Serruys et al., JANNUS: experimental validation at the scale of the atomic modelling, C. R. Physique (2007), doi:10.1016/j.crhy.2007.10.015

JANNUS
Joint Accelerators for Nano-Science & NUmerical Simulation

Modelling Oriented Experiments with Rapid Feedback

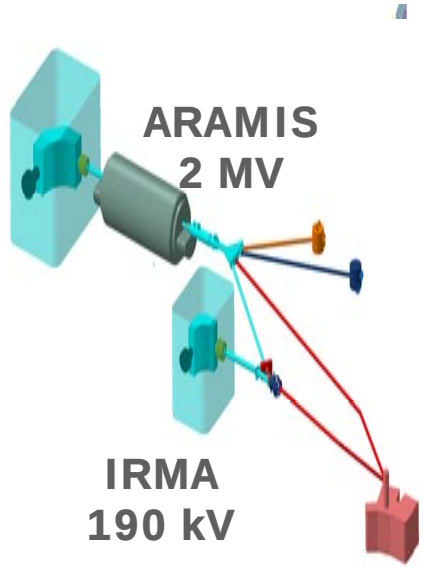
Triple beam : dpa and 2 implantations



Triple Beam
Single Beam
Ion Beam Analysis

Kinetic Pathway up to ~0.5T_M:
dpa & transmutation

In-Situ TEM : one beam (dpa, implantation)



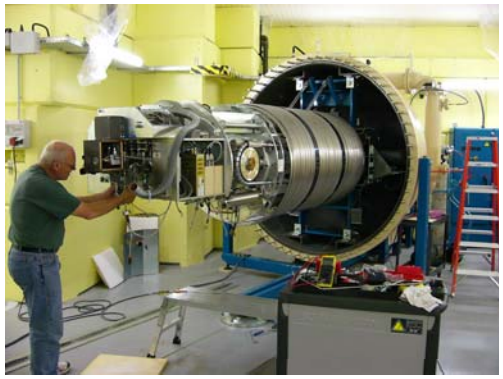
Single Beam Chamber
Ion Beam Analysis
On –line TEM

Point Defect Dynamics (<0.3T_M):
dpa and/or Implantation

Start of Operation as a Users Facility: Start 2009

Epiméthée 3 MV

- **Accelerator type:** Pelletron NEC (National Electrostatics Corporation
- **Tension :** 3 MV
- **Source :** ECR (Electron Cyclotron Resonance) Pantechnik
  - ⇨Multi charged ions: 1 <M< 209 200 keV <E< 60 MeV
- **Use :**
  - ✓Ballistic damage (until ~ 100 dpa/6 h)
  - ✓Beams H, D, He : Ion beam analysis or implantations



Available

Possible

Impossible

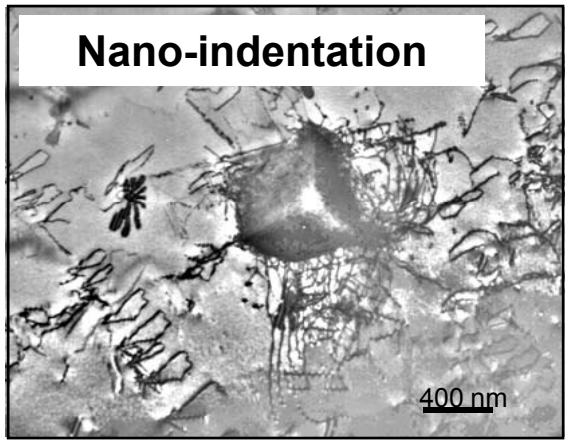
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac															

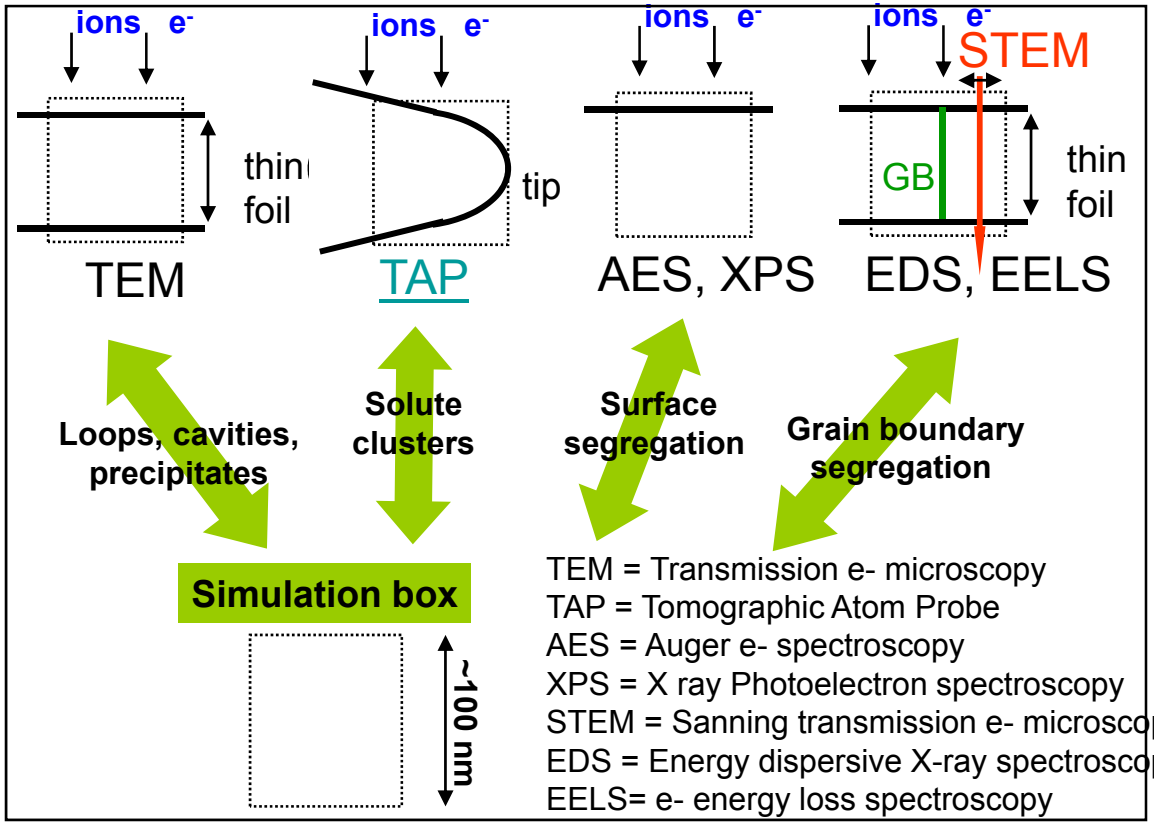
JANNUS : Modelling Oriented Irradiation & Characterisation

- Volume → experimental and simulated volumes are identical
- Surfaces → taken into account
- Flux and time conditions → explore wide enough ranges

Irradiation → **Charged particles: Dual Beam + in situ TEM, e⁻ VDG, HVTEM**

Direct observation → **Mechanical testing** → **Nano-indentation**





EFDA
EUROPEAN FUSION DEVELOPMENT AGREEMENT

JANNUS web site: http://jannus.in2p3.fr

instn DANS CSNSM JANNUS

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- Access to the platform
- Equipments
- Research topics
- Teaching and training
- Contact
- Request Beam time

JANNuS - Joint Accelerators for Nano-science and Nuclear Simulation

25 September, by Webmaster

The JANNuS (**Joint Accelerators for Nano-science and Nuclear Simulation**) multi-ion beam irradiation platform is a joint project between the **"Commissariat à l'Energie Atomique"** (CEA) through the "Direction de l'Energie Nucléaire" (DEN/DANS/DMN/SRMP) and the "Institut National des Sciences et Techniques Nucléaires" (INSTN), and the **"Centre National de la Recherche Scientifique"** (CNRS) with the "Institut National de Physique Nucléaire et de Physique des Particules" (IN2P3), and the **"Université Paris-Sud 11"** (UPS), through the "Centre de Spectrométrie Nucléaire et de Spectrométrie de Masse" (CSNSM).

The JANNuS platform includes **two experimental sites**:

- At CEA Saclay, **a triple ion beam facility** has been designed mainly for the simultaneous production by ion beams of nuclear recoil damage and concomitant generation of nuclear reaction products. Such a set of joint accelerators will provide users a facility, having no equivalent in Europe for well-controlled modelling-oriented experiments. These are needed to build the multi-scale modelling of irradiation effects in materials for nuclear applications. The facility is operating according to three modes: i) single beam (YVETTE or ÉPIMÉTHÉE for IBA measurement, ÉPIMÉTHÉE or JAPET for implantation/irradiation), ii) dual beam (ÉPIMÉTHÉE + JAPET or ÉPIMÉTHÉE + YVETTE or JAPET + YVETTE), iii) triple beam (ÉPIMÉTHÉE + YVETTE + JAPET).
- At CSNSM Orsay, **a 200 kV Transmission Electron Microscope is coupled with two ion accelerators** (ARAMIS and IRMA) for in-situ observation of the material microstructure modifications induced by ion irradiation/implantation. The facility is operating according to three modes: i) TEM + IRMA, ii) TEM + ARAMIS and iii) TEM in dual beam (IRMA + ARAMIS).

JANNUS

The overall JANNuS platform is designed to supply a large range of ion irradiation/implantation conditions, allowing in-situ Transmission Electron Microscopy (TEM) and ion beam analysis wit single, dual or triple beam combinations.

Request beam time

Access costs

The most recent articles

Call for Proposals Foreseen Twice a Year:

Fist One was in January 2009

DANS

What kind of Validation Experiments ? (2)

Various Neutron Spectra (see V. Voyevodin)

- **Material Testing Reactor: Macroscopic samples**
  - **Only dpa,**
  - **Too a low dose rate for DEMO**
- **Fast Neutron Reactors: Macroscopic samples**
  - **Only dpa,**
  - **Dose rate compatible with DEMO**
- **Spallation Target: macroscopic samples**
  - **Dpa + "too many" transmutation products,**
  - **Dose rate compatible with DEMO**

What kind of Validation Experiments ? (3)

A Neutron Source

with a prototypical spectrum:

- Dose rate
- Recoil Spectrum
- He/dpa and H/dpa

International Fusion Material Irradiation Facility:

IFMIF

The Fusion Materials Topical Group should be an important tool to select & optimise the IFMIF irradiation matrix

Neutron Sources to Simulate 14 MeV Neutrons

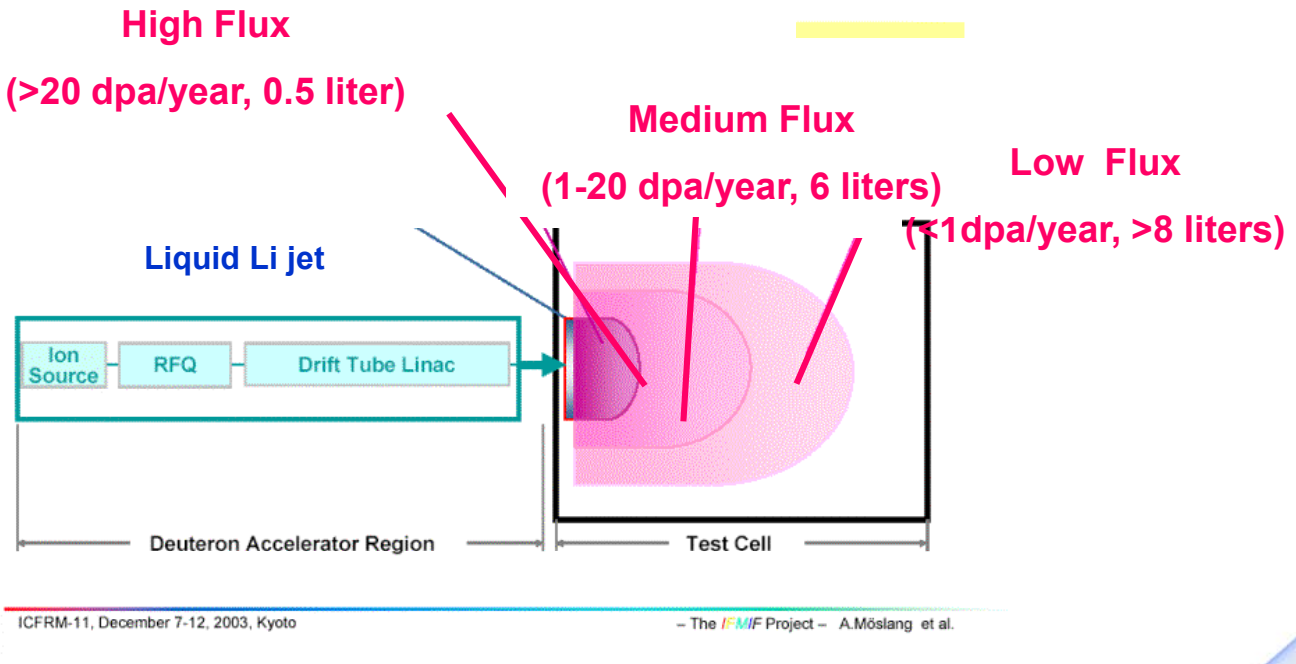
- Fission Reactors (MTR, Fast reactors), Spallation Targets
- International Fusion Materials Irradiation Facility (IFMIF)
  - Typical Stripping Reactions: $^{7}Li(D, 2n)^{7}Be$, $^{6}Li(D,n)^{7}Be$ $^{6}Li(n, T)$ 4He
  - Deuterons: 40MeV, 2x125mA, beam footprint 5x20 cm^2
  - EVEDA (in Japan): 2007-2012
  - Construction:2013-2018 –Operation 3 campaigns of 5 years each

IFMIF will have

the correct scaling in He & H production:

~12 appmHe/dpa

~45 appmH/dpa



Thank you very Much for your Attention