Helium Embrittlement:
Model of Helium Migration within Breeder Blanket Materials

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Motivation

Breeder blankets (BB) will be an essential part of DEMO. Located just behind the first wall of the reactor, breeder blankets have to withstand harsh conditions:

First Wall heat load	1 MW/m²
Neutron Wall Load	3 MW/ m²s
BB Proposed Lifetime	5 Years

Table 1: Journal of Nuclear Science and Technology Vol. 38, No. 11, November 2001 [1]

- EUROFER is one of the main contenders for materials used in breeder blankets.
- Helium cooled Pebble Bed and Helium cooled Lithium Lead are two reference blanket concepts for DEMO, which both use EUROFER.
- Design codes exist (RCC-MRx) for assessing ductile structures in high temperature environments and are integrating EUROFER their procedures.
- In DEMO, blanket materials are expected to be exposed to irradiation doses of > 70 dpa with operation temperatures < 550°C.
- Materials in breeder blankets can experience embrittlement through transmutation products.
- Work has been done to predict the timescales in which this phenomenon occurs. The current model neglects pinning mechanism such as dislocations, vacancies and voids.
- Models focus on modelling an iron lattice since this is the dominant element within steels.
- At temperatures < 550°C (823 K), iron is in α-phase, meaning it has a bcc structure.

Project Overview

- Construct simulations describing how helium moves through the matrix of the material.
- Use rate theory model to explore migration rates to grain boundaries (GB's) within α-Fe.
- Use density functional theory (DFT) data to validate the energies and parameters chosen for the model.
- Incorporate trapping mechanisms and impurity sinks into the model, which can act as pinning mechanisms for the helium.
- Incorporate the relation between helium nucleation and vacancy density.
- Use MD simulations to explore sink terms and coefficients for rate theory model.
- Determine the timescale at which helium reaches the critical helium embrittlement level at the grain boundaries and compare with previous embrittlement model.

Predicted Critical Helium Embrittlement Times

- The proposed steels for DEMO are composites crucially containing Fe.
- Model shows critical embrittlement lifetimes can be as low as 2 years with a given grain size (figure 1).
- Breeder blankets have a proposed lifetime of 5 years to reach economical viability.
- Model suggests that the time in which Fe becomes critically embrittled might fall short of the minimum of 5 years.
- The model makes use of the following formulas for determining the critical He concentration at GB:

$$G_{He}^{c} = \frac{3\nu_{He}^{c}}{an},\ \nu_{He}^{c} \approx \frac{2\varepsilon_{surf}}{E_{He}^{sol}}$$

- Once the G_{He}^{c} values have been found, MCNP is used to calculate the time scales on which it reaches these concentrations.
- Current models neglect He traps such as dislocations and voids.

Table 2. Table of calculated critical boundary densities ν_{He}^{c}, critical bulk concentrations G_{He}^{c} for He in various elements, and the approximate critical embrittlement-lifetimes t^{c} in DEMO full-power time and equivalent integral dpa. Results for two different grain sizes a shown.

				Critical times and dpa for GB embrittlement in DEMO			
				FW armour		blanket at depth of 17–19 cm	
Element	ν_{He}^{c} (cm^{-2})	a (μm)	G_{He}^{c} (appm)	t^{c}	dpa^{c}	t^{c}	dpa^{c}
Fe	6.90×10^{14}	5	48.8	4 months	4.79	2 years	9.57
V	6.75×10^{14}	5	56.1	1.5 years	25.07	7 years	41.52
Cr	5.52×10^{14}	5	39.8	5 months	6.27	2.5 years	12.75
Mo	8.05×10^{14}	5	75.3	2 years	19.12	10 years	31.26
Nb	7.41×10^{14}	5	80.0	2 years	31.99	10 years	51.61
Ta	7.77×10^{14}	5	84.1	19 years	107.60	137 years	304.17
W	9.16×10^{14}	5	87.2	20 years	88.89	228 years	357.37
Be	7.94×10^{14}	5	38.5	4 days	0.08	11 days	0.09
Zr	8.11×10^{14}	5	113.2	4 years	61.99	21 years	108.80
Fe	6.90×10^{14}	0.5	488.0	4 years	57.47	18 years	86.13
V	6.75×10^{14}	0.5	560.5	12 years	200.60	69 years	409.29
Cr	5.53×10^{14}	0.5	397.8	4 years	60.20	23 years	117.34
Mo	8.05×10^{14}	0.5	753.2	18 years	172.10	114 years	356.42
Nb	7.41×10^{14}	0.5	800.1	17 years	271.94	100 years	516.12
Ta	7.77×10^{14}	0.5	841.3	216 years	1223.20	> 300 years	>666.00
W	9.16×10^{14}	0.5	871.5	>300 years	>1333.00	>300 years	>470.00
Be	7.94×10^{14}	0.5	385.2	1 month	0.60	4 months	1.00
Zr	8.11×10^{14}	0.5	1131.7	37 years	573.39	217 years	1124.29

Figure 1. Calculated critical boundary densities, critical bulk concentrations and critical embrittlement-lifetimes. Nucl. Fusion **52** (2012) 083019 [2]

Trapping Mechanisms

- It was considered that dislocations (in particular edge dislocations) can act to increase the diffusion of helium interstitials down the dislocation core (pipeline diffusion). However, recent studies indicate that for light atoms, even with a low diffusion barrier down the core due to the large amount of free volume, the amount of free activation energy is 11-13 times higher than in bulk, amounting to diffusion much higher in bulk [3].
- Outside the core, around the dislocation, associated binding energies can facilitate helium nucleation around the dislocation, trapping the helium (figure 2).
- Vacancies and voids can also cause helium nucleation due to helium's high binding energy toward vacancy clusters.

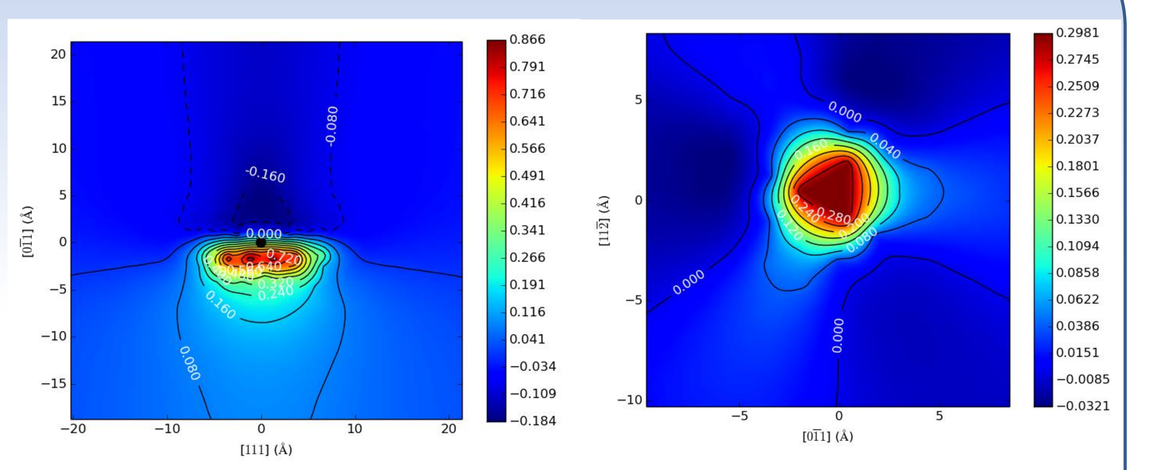

Figure 2. Binding energy map of an He interstitial to an edge (left) and screw (right) dislocation.

Rate Theory Model

- Rate Theory is a plausible method for determining the timescales in which helium migrates to the GB's and reaches the critical level of embrittlement.
- It uses transition state theory (which is often used in diffusion in solids and chemical kinetics) as a tool to determine the rates in which individual species interact with the surrounding system.
- It has been used for many years for understanding the processes involved in metals under nuclear irradiation.
- Data is often obtained from molecular dynamics and DFT [4].
- It comprises of kinetic equations that are tied into a master equation to produce a Size Distribution Function (SDF) (figure 3).
- The kinetic equations involve many terms, the main sink term of interest being the grain boundary sink.
- For every cluster size, a first order differential equation with several evolving terms exists, amounting to millions of equations to solve for every timestep.
- This is computationally impossible to do for the desired length of time with typical numerical methods.
- A grouping method has been proposed and used to reduce the amount of equations which still describes the behaviour to a good level of accuracy (figure 4) [5].

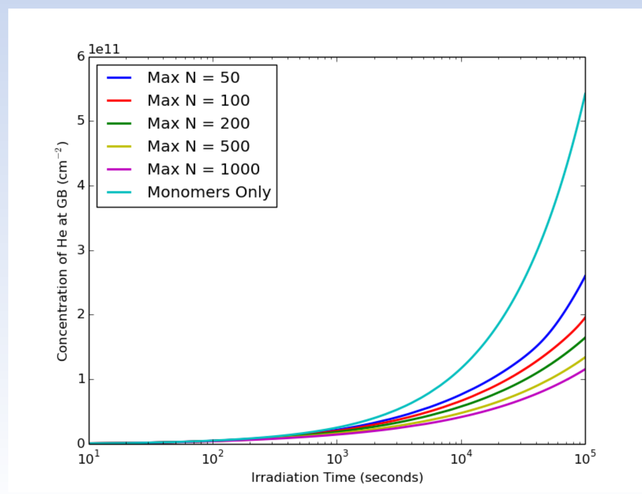

Figure 3. Concentration of helium at the grain boundaries with varying cluster size distributions after irradiation.

$$f(x) = L_0^i + L_1^i\left(x - \langle x\rangle_i\right).$$

$$\frac{\partial L_0^i}{\partial t} = \frac{1}{\Delta x_i}\left[J(x_{i-1}) - J(x_i)\right],$$

$$\frac{\partial L_1^i}{\partial t} = -\frac{\Delta x_i - 1}{2\Delta x_i \sigma_i^2}\left[J(x_{i-1}) + 2\langle J\rangle_i^* - J(x_i)\right].$$

Figure 4. Main mathematical terms for the new grouping method used for determining the size distribution function (f(x), where x is the number of interstitials or voids within the cluster) [6].

Conclusion

- Current models neglect internal obstacles within the grain, which can act to prevent helium from reaching the grain boundaries.
- With discovered trapping behaviour, more accurate helium nucleation and migration behaviour can be modelled on a large timescale.
- Observing behaviour of helium interaction with defects will reveal how the diffusion towards grain boundaries are effected.
- Using updated grouping method, it is possible to integrate this into rate theory models to obtain an updated estimate, for a given grain size, for the length of time for helium embrittlement to occur.

References

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