An Object Kinetic Monte Carlo model is being developed for dilute (less than 1% Cr) FeCr alloys. The model includes the effects of Cr on the mobility of radiation effects, using information obtained either from density functional theory or molecular dynamics calculations. The results are compared to experimental measurements of electric resistivity for different Cr concentrations. We analyse the dependence of Cr on the first two observed peaks: ID2 and IE and the influence of parameters such as the interaction radius between Cr and an Fe self-interstitial.

**Migrating species:**
- I up to size 4, V up to size 4
- ICr 0.23 eV
- LCr, ICr do not migrate

**Dissociation of clusters**
- \( \text{ICr} \rightarrow \text{I} + \text{Cr} \)
  \[ E = 0.08 + 0.34 = 0.42 \text{ eV} \]
- \( \text{ICr}_2 \rightarrow \text{ICr} + \text{Cr} \)
  \[ E = 0.08 + 0.23 = 0.31 \text{ eV} \]
- \( \text{ICr} + \text{Cr} \rightarrow \text{I} + \text{Cr}_2 \)
  \[ E = 0.394 + 0.34 = 0.73 \text{ eV} \]

**Simulation conditions**
- Electron irradiation at 77 K
- Isochronal anneal from 77 to 200K, Heating rate 3K/3min
- Pure Fe & FeCr at 0.019 at%, 0.047 at.% & 0.095 at.%

**Experimental results from Abe & Kuramoto [1]**

- Shift of stage IE to lower temperatures in FeCr
- Decreases in temperature and increases in amplitude with increasing Cr concentration
- Peak at 180K does not depend on solute concentration

**Conclusions:** The model reproduces the shift of stage IE towards lower temperatures when Cr concentration increases. This peak is related to the formation of ICr and ICr clusters. ICr migrates and recombines with V while ICr$_2$ dissociates into ICr and Cr. Since ICr migrates faster than an Fe interstitial the shift towards lower temperatures is reproduced. The position of the IE peak depends strongly on the ICr capture radius, with a capture radius of 0.28nm providing the best agreement with the experimental measurements. There is not a significative difference in the results when the I$_2$Cr and I$_2$Cr$_2$ reactions are not included. At least, at temperatures below 150K, the formation of these species does not seem to play an important role in defect evolution. Further work is underway to study the behaviour at higher temperatures.

**References:**

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