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The influence of carbon on point defect properties of proton irradiated Fe-Cr alloys

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Abstract

The effect of carbon on the point defect migration properties in Fe-Cr alloys with a concentration of 10 at.% Cr is studied by means of resistivity recovery measurements after low temperature proton irradiation. The presence of carbon mainly affects features of the resistivity recovery spectra in the temperature ranges of (a) 150 - 200 K, which are linked to self-interstitial defects, and (b) 400 - 500 K, which are probably due to vacancy complexes. The observations are discussed in terms of the possible interactions of carbon with radiation defects and its influence on solute atom re-ordering.

Keywords: resistivity recovery; point defects; carbon; Fe-Cr alloys; irradiation

1. Introduction

Carbon is one of the most important alloying element in steels playing a major role in the development of the microstructure and the mechanical properties. It has also a major influence on the irradiation behavior due its strong interaction with point defects. A number of experimental [1], [2] as well as theoretical [3], [4] works have elaborated on the strong influence of carbon impurities on the migration and annealing of point defects in iron. It has been shown that the formation of carbon-vacancy complexes is energetically favorable and, moreover, these complexes exhibit reduced mobility and may serve as nucleation sites for larger vacancy clusters and nanovoids. The interaction between carbon and self-interstitial atoms is also attractive but significantly weaker.

In the present work we investigate by resistivity recovery measurements the interaction between carbon atoms and radiation defects in Fe-Cr alloys, which are considered as model materials for the more complex ferritic/martensitic steels. This interaction is considered of key importance for the evolution of the microstructure of these steels during irradiation. We employ proton irradiation to introduce radiation defects and *in-situ* measurements of the electrical resistivity for assessing the associated radiation damage and recovery during subsequent post-irradiation annealing. The effect of carbon is revealed by comparing the recovery of carbon-doped and undoped Fe-Cr alloys of the same Cr concentration.

2. Experimental Methods

Two Fe-Cr alloys were obtained from EFDA with the composition shown in Table 1 as determined by chemical analysis. Both alloys contain about 10 at. % Cr while one of them is doped with C to a concentration of 0.38 at. %. The residual carbon content of the undoped alloy is approximately 20 appm. In the following the two materials will be referred to as Fe-10Cr and Fe-10Cr-C for the undoped and carbon-doped case, respectively. Specimens in the form of 50 μm thick foils were prepared by cold-rolling. The undoped specimens were annealed for 12hrs at 800°C under vacuum while the carbon doped ones were annealed for 1hr at 760°C to prevent carbon out-diffusion. Current and potential leads of pure Fe were spot-welded on the specimens for performing electrical measurements.

Table 1. Concentrations of alloying elements in Fe-Cr alloys (at. %)

Alloy Code	Cr	C	Other Impurities (O, N, P)
Fe-10Cr	10.8	0.002	0.004
Fe-10Cr-C	10.7	0.380	0.004

Irradiations were performed in the dedicated materials irradiation facility IR^2 at the TANDEM accelerator of NCSR "Demokritos" [5], which offers the capability of *in-situ* measurement of the electrical resistivity during and after irradiation. The samples were irradiated by a beam of 5 MeV protons, which have a range of approx. 80 μm in iron. Thus they penetrate fully the foil specimens and generate defects homogeneously within the irradiated volume. During irradiation the sample temperature was kept at 50 K by means of a closed-cycle helium refrigerator coupled to the accelerator beam line. At specific time intervals during the irradiation the proton beam was closed, the sample was cooled to 20 K and its irradiation induced residual resistivity change was measured. The beam flux, total dose and other details of the irradiation are given in Table 2. Recovery annealing up to 700 K was also performed *in-situ* without removing the sample from the irradiation chamber. The annealing temperature was increased in steps ΔT keeping a constant ratio $\Delta T / T \approx 0.03$. At each temperature step the annealing time Δt was such that $\Delta T / \Delta t = 1$ K/min. At the end of each annealing interval the sample was rapidly quenched to the base temperature of 20 K and the residual resistivity was measured. In this manner the recovery of radiation damage was monitored during annealing. Electrical resistance was measured with the standard DC four probe method using a constant current source and a sensitive nano-voltmeter (Keithley Inc). Current polarity reversal was used to eliminate thermal voltages. The resolution of the measurement system was 10^{-7} Ω.

Table 2. Conditions of the 5 MeV proton irradiation.

	Φ	$[\Phi \cdot t]_{max}$	dpa_{max}	ρ_i^0
	(cm^{-2} s^{-1})	(cm^{-2})	(ppm)	(μΩ-cm)
Fe-10Cr	2.0×10^{11}	2.7×10^{15}	~40	0.57 ± 0.03
Fe-10Cr-C	1.8×10^{11}	3.1×10^{15}		0.66 ± 0.03

Φ - beam flux; $\Phi \cdot t$ - fluence; ρ_i^0 - max. irradiation induced resistivity increase.

3. Damage generation

The irradiation induced increase of the electrical resistivity ρ_i is shown in Fig. 1a as a function of dose for both the pure and C-doped samples. The observed almost linear increase is due to the accumulation of radiation defects since at the irradiation temperature of 50 K their mobility is significantly reduced and there are no annihilation mechanisms. As it is seen from the figure, carbon does not have a significant effect on the damage generation. The experimental curves in Fig. 1a deviate slightly from a pure linear increase. This is more clearly seen in Fig. 1b, where the resistivity damage rate $\Delta\rho_i / \Delta[\Phi \cdot t]$ is depicted as a function of dose. The damage rate data of Fig. 1b are obtained by a point-by-point differentiation of the resistivity versus dose curves. The damage rate as a function of dose is well described by a linear relationship $A(1 - b\,\Phi \cdot t)$, where A and b are constants, which is depicted with the dotted line in Fig. 1b. The parameter A expresses the initial damage rate at zero dose and b quantifies the gradual decrease of damage rate. The best-fit values for the parameters are $A = (2.2 \pm 0.2) \times 10^{-22}\ \Omega\text{-cm}^3$ and $b = (2.7 \pm 0.5) \times 10^{-17}\ \text{cm}^2$, respectively. It is noted that the damage rate at the end of the irradiation is 10% lower than the initial one.

To estimate the amount of damage generated by the proton irradiation the SRIM code [6] has been utilized according to the recommendations of Stoller et al. [7]. In brief, SRIM is used to obtain the average damage energy T_{dam} and then this value is inserted in the NRT model of displacement damage [8] to estimate the number of atomic displacements. A displacement threshold energy of $T_d = 40\ \text{eV}$ has been used, which is the value typically used for Fe. The SRIM simulation predicts an average damage energy per displacement collision event, $T_{dam} = 300\ \text{eV}$. Thus, according to the NRT model a number of $0.8 T_{dam} / 2T_d = 3$ Frenkel pairs are generated per collision. Due to the low damage energy most of the collisions would result in the production of isolated Frenkel pairs and only a small fraction of defects will form larger clusters. Taking also into account the number of displacement collisions per ion from SRIM, the value of the damage cross section is found equal to $\sigma_d = 1.4 \times 10^{-20}\ \text{cm}^2$. Using this value it is estimated that the total concentration of Frenkel defects at the maximum dose shown in Table 2 is $N_{FP} = \sigma_d [\Phi \cdot t]_{\max} \approx 40\ \text{ppm}$.

The resistivity damage rate is equal to $\rho_F \sigma_d$, where ρ_F is the resistivity per unit concentration of Frenkel defects. Equating this to the experimental initial damage rate A it

is obtained that the apparent value of ρ_F is $(1.6 \pm 0.2) \times 10^{-2}$ Ω-cm in both undoped and C-doped Fe-10% Cr. Compared to the Frenkel pair resistivity of pure Fe $\rho_F(\text{Fe}) = (3.0 \pm 0.5) \times 10^{-3}$ Ω-cm [9] the value obtained here is 5 times higher. This is in agreement with previous results of Maury et al. [10] who observed an up to 6-fold increase of ρ_F in electron irradiated Fe-Cr alloys with a maximum Cr concentration of 3 at. %. These authors attributed the effect to the non-additivity of different conduction electron scattering mechanisms contributing to the total resistivity. This is also known as deviations from Matthiessen's rule and in ferromagnetic Fe alloys it is mainly due to spin dependent current conduction. In the case of irradiated Fe-Cr the scattering of conduction electrons from Frenkel defects and Cr atoms has different intensity in the spin-up and spin-down bands. This may account for the observed increase in the apparent resistivity per Frenkel defect as shown in [10].

Regarding the observed decrease of the damage rate with dose it can be either due to radiation annealing, i.e., the annihilation of already present radiation defects by new collisions occurring in their vicinity, or to the effects of spin dependent conduction discussed in the previous paragraph. Similar observations of diminishing damage rate in [10] have been attributed to deviations from Matthiessen's rule by Maury et al. However, the effect of radiation annealing cannot be excluded. Experimental data extending to sufficiently higher dose would be needed in order to discriminate between the two effects. It is noted that in the experiments of Maury et al. [10] the maximum radiation resistivity increase in the concentrated alloy Fe-3%Cr is only ~ 0.3 $\mu\Omega$-cm, i.e., about half of the total resistivity increase reached in the current irradiations.
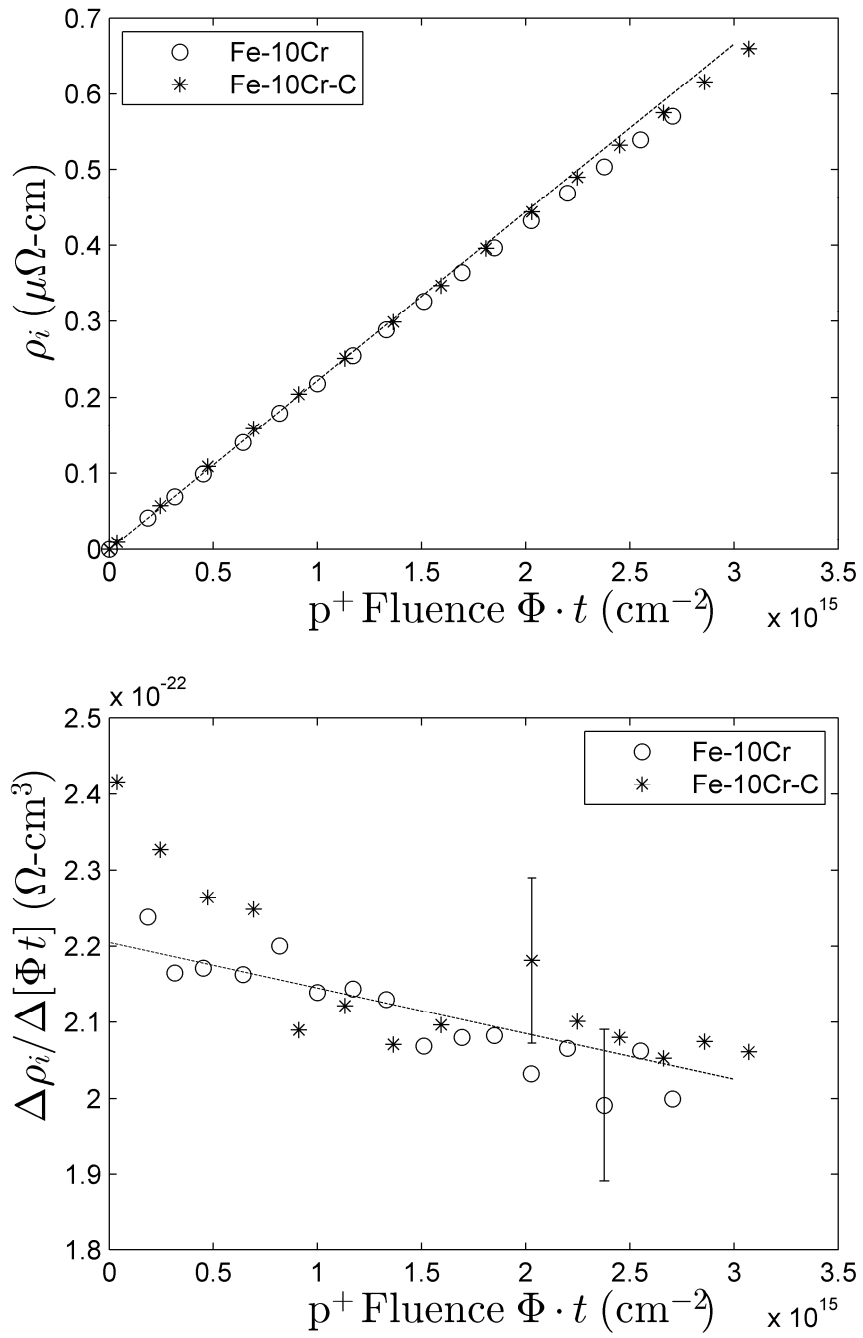
Figure 1. (a) Irradiation induced residual resistivity increase ρ_i and (b) resistivity damage rate as a function of dose in undoped and C-doped Fe-Cr alloys during proton irradiation at 50 K

4. Resistivity recovery
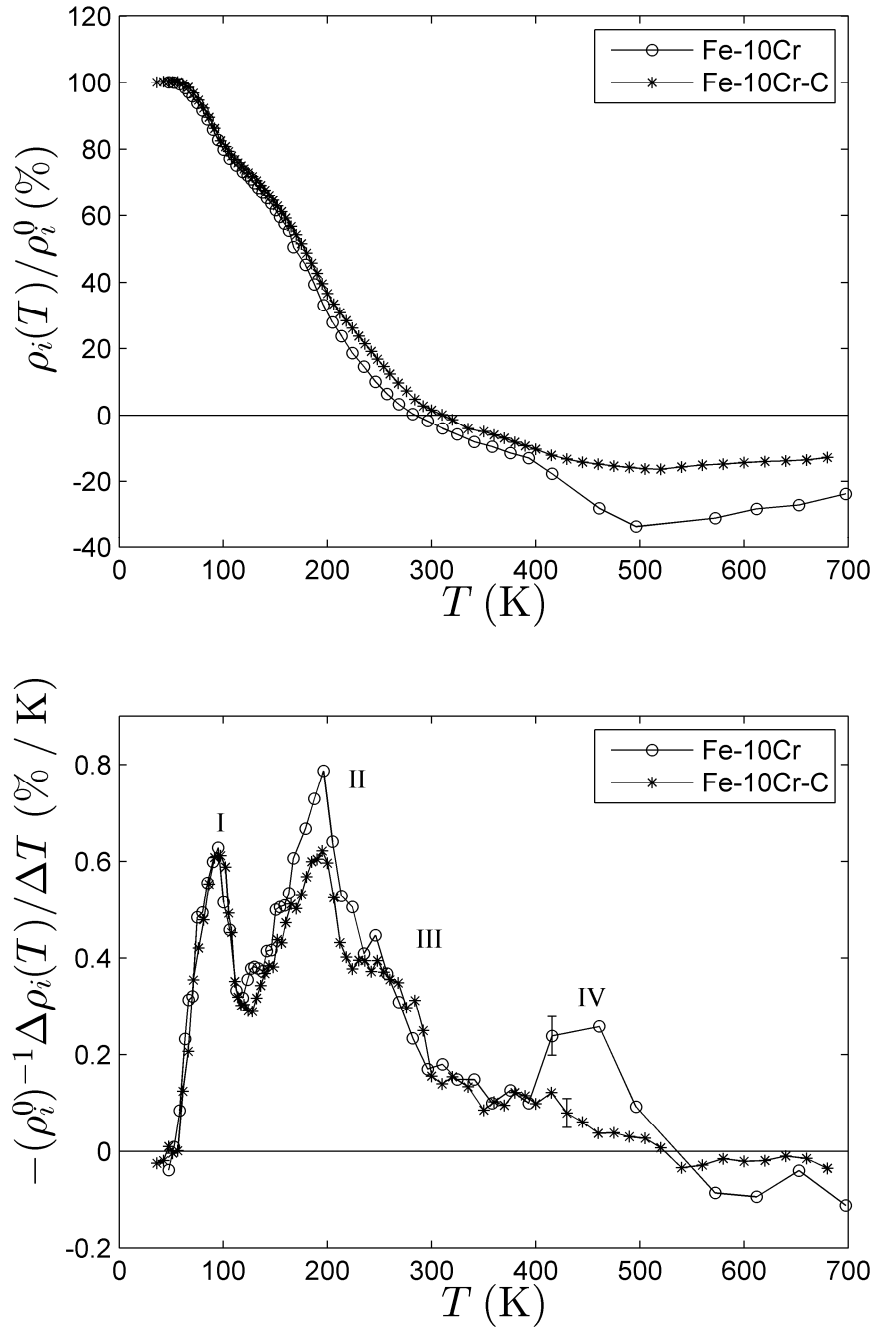
Figure 2. (a) Resistivity recovery and (b) recovery rate as function of annealing temperature for C-doped and undoped Fe-Cr alloys after proton irradiation at 50 K

Fig. 2a shows the resistivity recovery of the undoped and carbon-doped Fe-10%Cr alloy as a function of annealing temperature. The ratio $\rho_i(T)/\rho_i^0$, where $\rho_i(T)$ is the remaining resistivity increase at temperature T, reflects the fraction of radiation defects that survive after annealing at the given temperature. It is observed that the recovery proceeds similarly

in the two materials, however the presence of carbon slows down the recovery process in Fe-10Cr-C above about 200 K. Notably, in both materials the resistivity recovery becomes negative, i.e., the resistivity of the samples becomes lower than their pre-irradiation value. This effect is more pronounced in the Fe-10Cr alloy in the temperature range above 400 K. It is noted that this effect is observed only during post-irradiation annealing. Annealing of un-irradiated Fe-10Cr and Fe-10Cr-C samples in the temperature range 300 - 600 K does not result in significant changes of the residual resistivity. Thus the observed resistivity reduction is associated with the annealing of radiation defects.

In fig. 2b the recovery rate $-(\rho_i^0)^{-1}\Delta\rho_i(T)/\Delta T$ is presented as a function of annealing temperature. $\Delta\rho_i(T)=\rho_i(T)-\rho_i(T-\Delta T)$ represents the difference in remaining resistivity increase between two successive annealing temperatures separated by ΔT. Plotting the recovery rate assists in the identification of temperature regions of intense recovery that may be associated with different defect reactions. The curves in Fig. 2b show four distinct maxima, or recovery stages, labeled from **I to IV**. The temperature of the maximum $\hat{T}$ (K) and the total recovery A (%) associated with each stage are listed in Table 3. The quantity A represents the integrated area beneath a recovery peak in Fig. 2b.

From the data of Fig. 2a it is obtained that at the annealing temperature of 500 K the fractional recovery is equal to -16 and -34 %. Such negative values in the recovery curves of concentrated alloys after irradiation have been frequently observed in the past [11], [12] and have been typically attributed to solute atom re-ordering taking place during the migration of radiation defects. In Fe-Cr alloys with a Cr concentration close to 10 at. % as in the current experiments, a resistivity reduction of ~10 % has been observed after electron irradiation to a total $\Delta\rho_i^0=0.56$ μΩ-cm and annealing to 300 K [13]. This is comparable to the magnitude of the reduction observed here in Fe-10Cr after annealing at temperatures slightly above 300 K. On the other hand, only a minor resistivity reduction has been observed after electron irradiation to a total $\Delta\rho_i^0=3.2$ μΩ-cm and subsequent annealing to 600 K [14]. The absence of resistivity reduction in [14] must be due to the much higher irradiation induced resistivity $\Delta\rho_i^0$ and the associated higher damage level. The resistivity recovery is then dominated by the contribution of defect annealing and the effect of solute atom ordering is completely masked. Fe-Cr is known to exhibit short-range ordering at concentrations below about 10 at.% and short-range clustering above this concentration [15], [16]. Furthermore, it has been observed that the resistivity of Fe-Cr at a Cr concentration of 10 at. % is slightly reduced during annealing at temperatures above 700 K

due to the re-ordering of solute atoms. This resistivity reduction becomes more pronounced at higher Cr concentration where short-range clustering of Cr occurs [15]. Thus, the negative recovery values observed here are attributed to a weak short-range clustering of Cr atoms that occurs via the migration of irradiation defects. The fact that this effect is reduced in the C-doped alloy could be explained either (a) by a coupling of carbon to the defects responsible for Cr clustering with an associated reduction of their mobility or (b) by a interaction between carbon and Cr that effectively prevents Cr clustering.

Table 3. Resistivity recovery stages. Maximum temperature $\hat{T}$ and total recovery A of resistivity stages

Stage		Fe-10Cr	Fe-10Cr-C
I	$\hat{T}$ (K)	95±2	95±2
	A (%)	30±2	30±2
II	$\hat{T}$ (K)	195±3	195±3
	A (%)	55±3	46±3
III	$\hat{T}$ (K)	240±5	260±5
	A (%)	26±3	30±3
IV	$\hat{T}$ (K)	450±10	400±10
	A (%)	23±2	11±2

The effect of carbon on the resistivity recovery is more clearly revealed in fig. 2b where it is observed that carbon affects mainly stages II and IV. There is no effect of C on stage I and only a slight influence on stage III. According to the current understanding of recovery processes in Fe-Cr from previous experimental [10], [13], [14], [17] and theoretical [18]–[20] work the following conclusions are drawn from the observed effect of carbon on the recovery stages.

Stage I. This stage is attributed to the correlated recombination of Frenkel defects by the migration of self-interstitial atoms (SIA) to their respective lattice vacancies. Despite the high carbon concentration of the Fe-10Cr-C alloy there is no observed effect of the carbon atoms on the correlated recovery. This is surprising since it is known that C impurities act as a traps for interstitial defects in Fe [2]. However, the migrating SIAs would react mainly

with the carbon that is dissolved in the Fe matrix and this is at most equal to the carbon solubility in ferrite, i.e., ~ 0.1 at. % at the annealing temperature. This would correspond to an average distance of at least $\sim 8a_0$ between carbon atoms, where a_0 is the lattice constant. This is much larger than the average migration distance for correlated SIA-vacancy recombination, where the SIA migrates towards its own vacancy. This is of the order of 1 lattice constant in Fe [2] and it is not expected to increase much in Fe-Cr alloys. On the other hand, as has been discussed by several authors [17], [19], [20], SIAs in stage I of Fe-Cr are primarily trapped by Cr atoms and this effect masks any possible influence of C.

Stage II. This stage is attributed to the release of SIA defects from Cr traps that captured them during stage I migration. According to [20], this trapping occurs with an average binding energy of 0.4 eV. The interstitials are detrapped at higher temperature leading to the occurrence of stage II in the temperature range 150 - 200 K. The maximum of stage II is observed here at $\hat{T} = 195\ \mathrm{K}$, both in the undoped and C-doped alloys, in agreement with previous observations in Fe-Cr [14]. However the presence of C has a significant effect on the total recovery in stage II, which is reduced by about 10% (cfg Table 3). This may be explained by two different mechanisms. First, it could be assumed that a fraction of SIAs released from Cr traps in stage II are immediately re-trapped by C atoms. The capture of SIAs by carbon impurities has been shown in pure Fe [2]. However, this would require the carbon-SIA complex in Fe-Cr to have a higher binding energy than 0.4 eV in order to survive stage II recovery. A different explanation can be offered by solute atom re-ordering effects. Since a significant fraction of SIAs in Fe-10Cr are mixed Fe-Cr dumbbells [19], the transport of Cr atoms is possible during their migration. This could allow the weak clustering of Cr to already start at stage II and thus a part of the resistivity recovery in this stage to be actually due to this clustering and not to defect annealing. In recent experiments in Fe - 5 at. % Cr [21] it has been shown indeed that ordering reactions at this Cr concentration start already in the temperature range of stage II. Thus, the observed reduction of stage II amplitude by C may be attributed to the obstruction of solute clustering.

Stage III is generally associated with vacancy migration, both in Fe-Cr alloys [14], [20] as well as in pure Fe [2]. Given the strong interaction between vacancies and carbon atoms in Fe [1], [2] it is surprising that this stage is only slightly affected by the presence of carbon in the Fe-10Cr-C. This can be understood if one considers the actual amount of defects that survive after stage II. According to table 2 the fraction of defects is ~15% in Fe-10Cr,

which corresponds to a concentration of 6 appm. This is even below the residual C content of the undoped Fe-10Cr alloy (20 ppm) and shows that already in the undoped alloy, vacancy migration may be dominated by the presence of carbon. Thus stage III in both C-doped and undoped samples is due to the same physical mechanism, namely, to the capture of vacancies by carbon impurities and the formation of vacancy-carbon (V-C) complexes, similar to what is observed in pure Fe [1], [2] .

Stage IV. This stage is clearly related to Cr clustering effects since a large part of the negative recovery in Fe-10Cr is developed within the temperature range of this stage, 400 - 500 K (cfg. Fig. 2a). It is noted that stage IV has not been observed in previous resistivity recovery experiments on electron irradiated Fe-Cr alloys of the same Cr concentration [14] probably due to the much higher irradiation dose that, as discussed above, tends to mask solute ordering contributions. Despite its relation to Cr re-ordering, the presence of stage IV shows also that a defect is definitely undergoing migration or dissociation in this temperature range, at the same time facilitating the clustering of Cr. Furthermore, the suppression of stage IV in Fe-10Cr-C shows that C inhibits this process. The defect involved in stage IV could be most probably identified as the one that forms during stage III, i.e., the V-C complex. Then stage IV in Fe-10Cr would be due to dissociation of this complex, a process that in pure Fe in known to occur at temperature above 500 K but may be shifted in Fe-Cr due to a reduction of the binding energy. The suppression of stage IV in the C-doped alloy can then be explained by the further decoration of V-C by mobile carbon atoms to form $V-C_2$ complexes. Theoretical calculations show that these are more stable in Fe [3], [4] and this stability relative to V-C may be retained in Fe-Cr alloys. Thus in Fe-10Cr-C a number of vacancies remain bound in $V-C_2$ complexes at the of the annealing.

5.   Conclusion

The interaction of carbon with irradiation defects has been studied in Fe-Cr alloys with a 10.7 at. % concentration of Cr. Samples of this alloy doped with 0.38 at. % of carbon as well as undoped were irradiated with 5 MeV protons in the low dose and low temperature regime. The effect of carbon was revealed during the subsequent measurement of the resistivity recovery. It was observed that the presence of carbon affects mainly the stages II and IV of the recovery spectrum. This has been attributed to trapping of SIA defects by carbon atoms during stage I and to the suppression of ordering effects in stage IV by

carbon. Carbon does not have any observable influence on the damage generation and the initial SIA migration stage.

6. Acknowledgements

7. References

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