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Damage buildup and edge dislocation mobility in equiatomic multicomponent alloys

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Abstract

A new class of single phase metal alloys of equal atomic concentrations has shown very promising mechanical properties and good corrosion resistance. Moreover, a significant reduction in damage accumulation during prolonged irradiation has also been observed in these equiatomic multicomponent alloys. A comparison of elemental Ni with the two component NiFe- and the three component NiCoCr-alloy showed a substantial reduction in damage in both alloys, and an even larger difference was seen if only larger clusters were considered. One of the factors limiting the damage build-up in the alloys compared to the elemental material was seen to be dislocation mobility [Physical Review Letters 116, 13 (2016) 135504]. In this Article, we focus on a more thorough investigation of the mobility of edge dislocations in different cases of the Ni-, NiFe- and NiCoCr-samples. We find that even though the saturated amount of defects in the alloys is lower than in elemental Ni, the defect buildup in the early stages is faster in the alloys. We also find that the dislocation mobility in NiFe is lower than in Ni, at low stresses, and that the onset stress in NiFe is higher than in Ni. The same phenomenon was seen in comparison between NiFe and NiCoCr, since the three component alloy had lower dislocation mobility and higher onset stress. The dislocation velocity in elemental Ni plateaued out just under the forbidden velocity, whereas the alloys showed a more complex behaviour.

Keywords: dislocation, molecular dynamics, mobility, equiatomic, multicomponent, alloy
PACS:

1. Introduction

In the search for materials to be used in harsh conditions or that can be utilized longer due to improved wear resistance, a new class of materials, so called High Entropy Alloys (HEA), have shown many good properties [1, 2, 3, 4, 5, 6].

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These alloys are a random mix of many elements of large fractions, in contrary to normal alloying where there usually is one base metal and many alloying elements in small fractions. A sub-category of HEA is multicomponent alloys, these alloys contain large fractions of several elements, but less different elements than in normal HEA. Another sub-category is equiatomic multicomponent (EAMC) alloys, that are similar to multicomponent alloys, but the fraction of the used elements are equal. Both HEA and the multicomponent alloys have shown promising mechanical properties [3, 4] and good corrosion resistance [4]. Recent studies have shown that the multicomponent alloys also show reduced defect accumulation, both experimentally and computationally, during continuous irradiation [5, 6]. The reduced accumulation of defects in the alloys indicates that they may be used in future nuclear power plant concepts, where irradiation is present and the environment could be corrosive [7].

It was recently shown that dislocation mobility was one of the key factors to the reduced defect accumulation in the EAMC alloys [5]. The reduced dislocation mobility hindered the formation of large dislocation structures, and therefore reduced the amount of retained defects in the alloys. The movement of dislocations also determines the mechanical properties of metals, which are crucial to know in order to use these new alloys as structural materials. In this Article, we present more detailed analysis of the previously obtained data in Ref. 5, on the defect accumulation in the EAMC alloys. We also study more thoroughly the mobility of edge dislocations in these alloys and compare them to the elemental Ni.

2. Methods

To investigate the mobility of edge dislocations, we used the classical molecular dynamics code PARCAS [8, 9]. The atomic interactions for Ni and NiFe were described by the interatomic potential by Zhou *et al.* [10]. To describe the NiCoCr alloy, we added the Lin *et al.* Cr-potential [11] to the potential for NiCo by Zhou *et al.* The Cr potential was joined to multi-elemental potentials from Ref. 10 by taking the Cr potential in the same formalism by Lin *et al.* [11]. To describe the interactions between the different elements in this system, we used the mixing scheme proposed in Ref. 10 between all the elements Ni-Co-Cr. However, this mixing rule did not work well for the Cr potential made with a different shape [11]. Hence for the mixed Cr-X potentials we used the mixing rule between the other elements and Fe, which has the same crystal structure and almost exactly the same lattice constant as Cr. The Cr-Cr interaction and Cr embedding energy were the original ones [11]. These same potentials and the same simulation code were used in the original study of the defect buildup simulations during massively overlapping cascades in the EAMC alloys [5]. In Ref. 5 the details of the simulation technique is described.

For the dislocation mobility study we used a simulation cell with the axis oriented along the [110], $[\bar{1}1\bar{2}]$ and $[\bar{1}11]$ directions, for the x-, y- and z-directions, respectively. The dimensions of the simulation cell were 30 unit cells in the x-direction, 100 unit cells in the y-direction and 20 unit cells in the z-direction.

This resulted in a simulation cell with the size $25 \times 13 \times 12$ nm^3, containing around 360000 atoms. We used periodic boundary conditions in the x- and y-directions, which lead to a 13 nm long segment of the edge dislocation with an unique surrounding. To obtain the dislocation in an FCC crystal, we cut out a one unit cell thick slab in the x-direction from the bottom up to the half of the cell. This will result in N layers in the upper half and N - 1 layers in the bottom half. The two halves were then compressed and extended by the Burger's vector divided by two, to obtain a rectangular cell containing a dislocation [12]. This cell was then relaxed for a few picoseconds to reach equilibrium, before a shear stress was applied to the cell. To investigate the movement of the dislocations, a few layers of atoms at the bottom were fixed and a constant force in the x-direction was applied to a few layers of atoms at the top. This force induced a shear stress $\sigma_{xz} = \frac{\mathbf{F_x}}{A_{xy}}$. To keep the temperature around 300 K, we used a Berendsen thermostat on a few layers of atoms above the fixed bottom atoms [13]. This was the same temperature of the sample as in the previous experimental and computational study.

We investigated three different materials, elemental Ni, NiFe- and NiCoCr-alloys, and obtained their edge dislocation velocities at different applied constant shear stresses. We investigated three different random atomic configurations for the NiFe- and NiCoCr-alloys, and three cases with different seeds for the elemental Ni samples. We simulated the movement up to 1 ns, for the lower stresses, to see the possible movement in the alloys. To obtain the average velocity of the dislocations, we started by determining the HCP atoms in the stacking faults between the two partial dislocations by an Adaptive Common Neighbor Analysis in OVITO [14]. The position at a given time was determined as the center of the HCP atoms, and by calculating the average movement between frames, we obtained the average velocity when the dislocation showed a steady movement.

3. Results and Discussion

In the previous study by Granberg *et al.* [5], the accumulated defect amount was investigated by Wigner-Seitz analysis at the different doses for the overlapping cascades. In that study, it was seen that the amount of defects was lower in NiFe compared to elemental Ni, and that the amount of defects in NiCoCr was a bit lower than in NiFe. These individual results are shown with the average curve fit in Fig. 1, where we can see the fluctuations in the single sample results. In this graph, each thin line of the same color represents the same alloy, but of different random composition/initial seed. The thick lines are the fit to the averaged data. Fig. 1 demonstrates strong fluctuations in the amount of defects for the individual simulations. These sudden increases and decreases are explained by the appearance of large defect structures and dissolution of defect clusters, reflected in large fluctuations within short times. Even though the alloys show a lower amount of defects when saturated, we, however, observe during the beginning of the irradiation that the amount of defects are rising

faster in the alloys compared to the elemental Ni (see Fig. 2). For instance, at 0.008 dpa we see 147 ± 11 defects in Ni, 233 ± 17 in NiCoCr and 243 ± 35 in NiFe in the simulation cell of 108000 atoms. In individual keV cascades in metals (not overlapping previous damage), the final damage structure is widely acknowledged to be due to the kinetics of the recrystallization phase of a heat spike [8, 15, 16, 17]. During this recrystallization, vacancies are pushed towards the center of the heat spike. In the metal alloys, the vacancy formation energy must vary for different nearest-neighbour element compositions, and hence the probability for 'leaving a vacancy behind' can increase for those compositions that happen to lead to a lower vacancy formation energy than in pure elements. This can explain why in the low-fluence limit, more damage is produced in the alloys than in the pure elements.

Next we turn to the more complex question of why at high doses ($\gtrsim 0.1$ dpa) the trend reverses and there is less damage in the alloys. In Ref. 5 this was attributed to dislocation mobility, but no data on that was presented.

The edge dislocation velocities for the different samples are shown in Fig. 3, where the average velocity of the three different samples are shown. The filled symbols represent the average value, for all three samples where the steady movement of the dislocation was observed, and the open symbols are the average for those where only 1 or 2 cases showed constant movement. The step like movement at some lower stresses are described later in the text. The results show that the dislocation velocity at lower stresses is much higher in elemental Ni compared to the alloys. The edge dislocation in Ni can move at all applied forces, but the dislocation in NiFe requires a higher stress to reach steady movement. If the two component alloy, NiFe, is compared to the three component alloy, NiCoCr, it is seen that the three elemental alloy will require even higher stresses to obtain steady movement.

We observe that the velocity plateaued for elemental Ni between 1900 m/s and 2000 m/s, which is similar to previous studies, where the velocity reached a maximum just under the forbidden velocity defined by the continuum elasticity [18]. For the two element alloy NiFe we see that the velocity starts to plateau, but then jumps to a similar velocity plateau as for the elemental Ni, but when the stress is increased the velocity jumps to the next plateau. For the three elemental alloy NiCoCr we do not see any discrete steps or plateauing, as the velocity increases continuously with an increasing stress.

At the lower stresses the behaviour is quite different between the different samples. The edge dislocation in elemental Ni can move at all investigated stresses, but for the alloys the different samples show different behaviour. This description is presented in Tab. 1. For NiFe one of the three cases started to move continuously at 46 MPa and two of the three cases at 58 MPa. At 70 MPa all of the dislocations did move continuously in NiFe. In the three element alloy NiCoCr one moves continuously at 145 MPa, and all move continuously at 175 MPa. In NiFe, at stresses between 23 MPa and 58 MPa the movement is not continuous. In most cases a movement of half a cell or once through the cell was observed and after this movement the dislocation is stuck for the rest of the simulation. For the initial structure that will move at 46 MPa, the dislocation

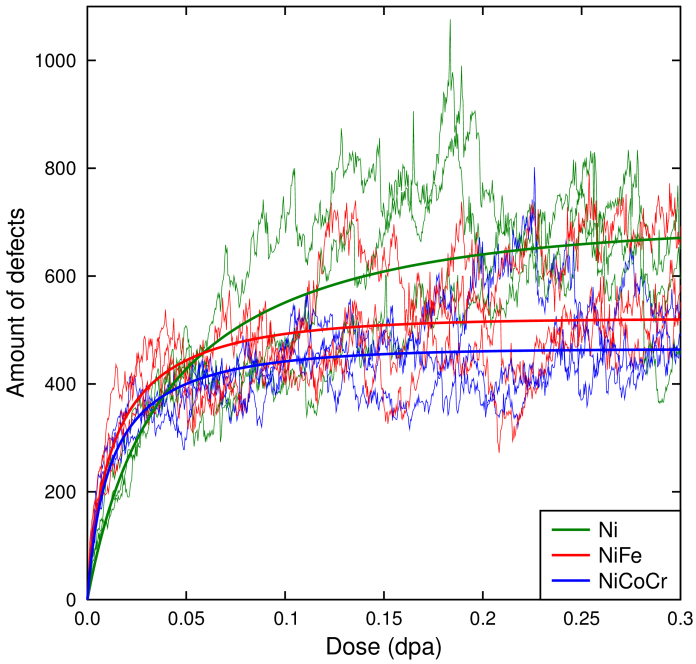

Figure 1: The amount of defects at different doses for each of the three different cases, where the thin lines are the single cases and the thick line the fit to the averaged data.

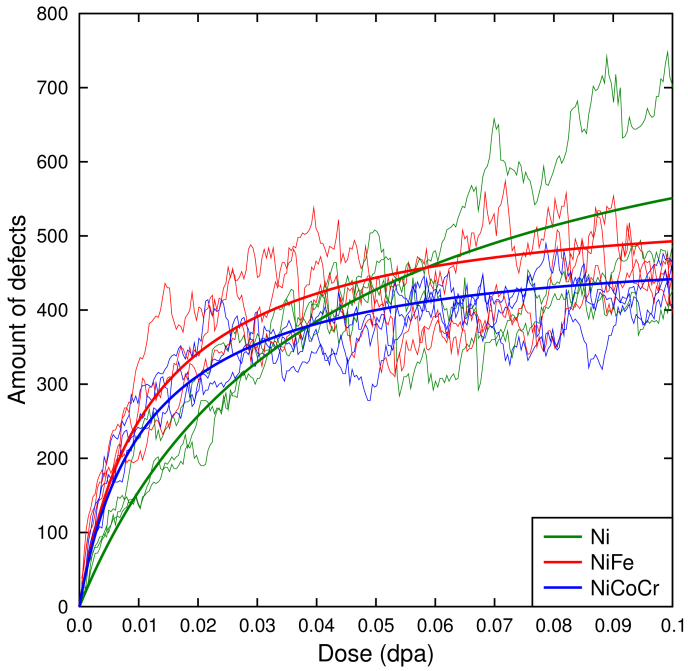

Figure 2: A zoom in of the beginning of the defects at different doses, where the thin lines are the single cases and the thick line the fit to the averaged data.

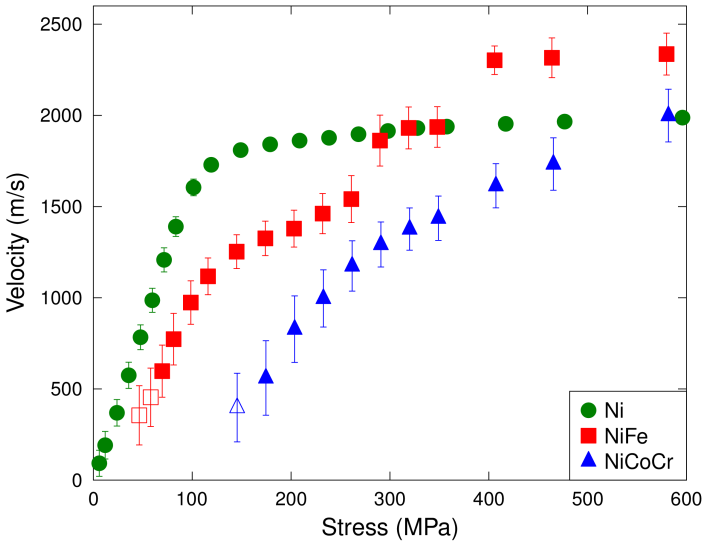

Figure 3: The obtained dislocation velocities at different applied stresses.

	Ni	NiFe	NiCoCr
6 MPa	3x		
12 MPa	3x	-	-
23 MPa	3x	o	-
46 MPa	3x	1x	
58 MPa	3x	2x	-
70 MPa	3x	3x	
116 MPa	3x	3x	o
145 MPa	3x	3x	1x
175 MPa	3x	3x	3x

Table 1: Detailed analysis of the behaviour of the edge dislocations, where the stresses are listed when a change has happened. A number plus an "x" is the amount of cases that reached steady movement at the given stress (out of three cases studied). An empty space is data that was not investigated in this study and a "-" means that the dislocations did not move at all during the 1 ns simulation. An "o" means that at least one dislocation did move, but did not reach steady movement.

moves a few times through the cell before it is stuck at 35 MPa. For NiCoCr, the dislocations do move either only a bit and then get stuck at 116 MPa to 145 MPa, or move continuously for a while and then get stuck for a longer time before they may continue to move. This indicates that the varying local environment of the dislocation can pin the dislocation for the whole simulation time, or for a shorter time and overcome the environment by thermal activation. To obtain an average velocity for these cases would be very unreliable. However, we note that it is possible for the edge dislocations to move at lower stresses than the values given here, since on time scales longer than those available in MD simulations, the dislocation motion will be thermally activated.

4. Conclusions

In this Article, we have determined the edge dislocation mobility for two equiatomic multicomponent alloys and compared the obtained results with elemental Ni. We observed that the edge dislocation can move at room temperature at all the investigated stresses in the elemental Ni, whereas the alloys showed a different behaviour. Both alloys required a higher stress to obtain a steady dislocation motion, and at a given stress, the velocity was lower in NiFe than in Ni and in NiCoCr it was still lower than in NiFe. At stresses lower than those to obtain steady motion, we observed some ill defined movement of the edge dislocation in the alloys. This steplike motion or a steady motion and a sudden stop indicates the effect of local environment: some atomic configurations can pin the dislocation, and keep the dislocation stationary on a MD timescale.

We also showed that even though the amount of accumulated defects in the alloys are lower than in the elemental sample, the total amount of defects is higher in the beginning of the irradiation. This is attributed to the alloy

structure slowing down point defect motion, which can reduce the defect recombination in single cascades.

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