IMPROVED RADIATION RESISTANCE IN EQUIATOMIC MULTICOMPONENT SINGLE PHASE ALLOYS

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The conventional metals are well-ordered crystal structures, with additional elements mixed in at small concentrations. A conceptually new way of making to mix numerous (three to seven) different types of metal atoms at completely random positions in equal concentrations, while still retaining a single crystalline phase. In these, so called equiatomic or high-entropy alloys, the atoms are thus completely disordered in position.

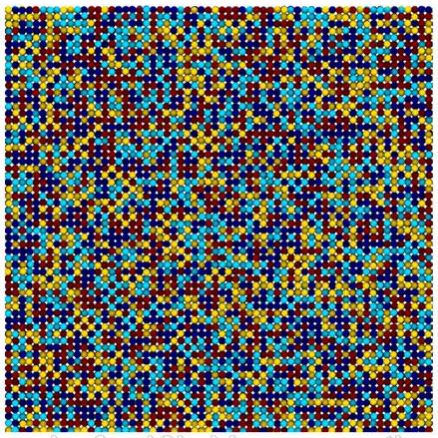

Fig.1 Single phase concentrated 5-element alloy with randomly ordered species.

Even though a metal with high degrees of disorder like high-entropy alloys might not at first appear like a good candidate to avoid radiation-induced disorder, however, it can be seen the other way around: the high level of disorder may in fact prevent the disorder level from increasing. Combining simulations and experiments we have recently shown [1,2] that atom-level disorder in NiFe and NiCoCr alloys, compared to elemental Ni, indeed lead to a substantial reduction of damage accumulation under prolonged irradiation. The random arrangement of multiple elemental species lead to unique site–to–site lattice distortions, that slow down the motion of extended defects, known as dislocation formed by the irradiation. This, in turn, lead to slower growth of large dislocation loops, which are the dominant form of radiation damage in metals at high doses. The examples of damage buildup in Ni and NiCoCr after the same irradiation dose of 0.3 dpa are shown in Fig.2. These simulations were performed by running 5keV recoil cascades in started at random positions within the simulation box. The

cascade was allowed to develop for 300 ps with the border cooling only, and after that, the excess of energy was scaled down to the room temperature by applying the Berendsen thermostat to all atoms in the box. The details of the simulations can be found in [1,3]. Here one can see the large dislocation loops in Ni absorbing smaller dislocation formations, while the population of small dislocation loops is almost intact in NiCoCr. Understanding of alloying effects on modified energy landscapes in such chemically disordered single-phase alloys will allow prediction of radiation-tolerance alloys for next-generation nuclear reactors and other high-radiation environments.

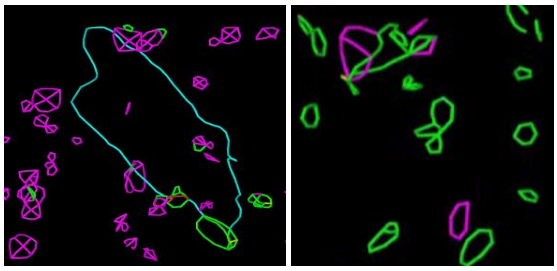

Fig. 2 Damage buidup in pure Ni (left) and NiCoCr (right) after 0.3 dpa irradiation dose.

The analysis also revealed that alloying effects on significant reduction of dislocation mobility is generic, and not specific to the current choice of materials or number of elements in the system. The large improvement from Ni to NiCoCr demonstrates that a reduction will depend on material choice, and suggests that there may be alloys with even larger damage reduction than the currently observed one – especially in more chemically disordered alloys with increasing number of principal elements at significant concentrations, where the number of possible

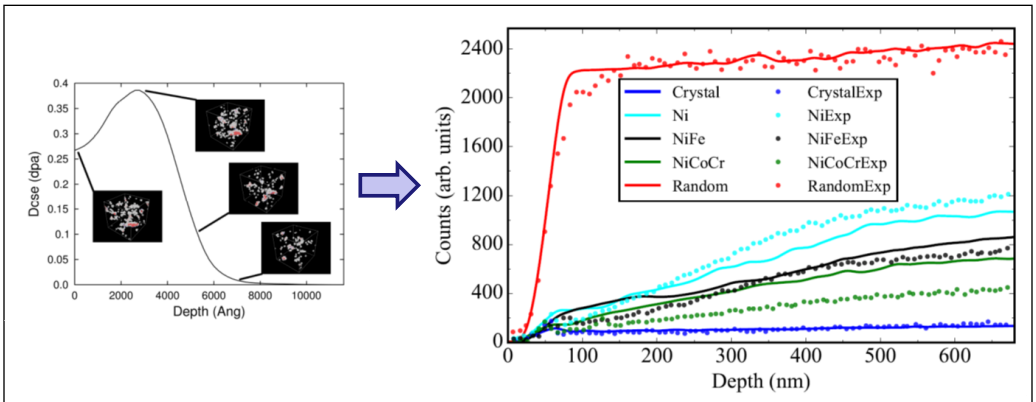

Fig.3 Simulation cells are subsequently selected to correspond to the damage level generated by irradiated ions along the path. The sequence is selected as shown in the diagram to the left. This way a sample of experimental size can be reconstructed. The comparison of RBS/C spectra from an experiment samples and corresponding simulation models, reconstructed from molecular dynamics simulations, shows a very good agreement without use of any fitting parameters. For more details see [5].

element combinations and alloy compositions are practically limitless.

To enable the direct comparison of simulation results with experiment, we developed a new method using binary collision approximation to simulate the Rutherford backscattering spectra in channeling conditions (RBS/C) from molecular dynamics atom coordinates of irradiated cells [4]. In this approach, a simulation of damage buildup in a single simulation cell was used to select the frames at the time when the irradiation dose reached the value corresponding to the damage depth profile in experimental samples (see Fig.3 to the left). Built on top of each other, these frames form a single sample with the damage distribution depth profile close to the one observed in the experiment. The approach allows comparing experimental and simulated RBS/C signals as a function of depth without fitting parameters. The simulated RBS/C spectra of irradiated Ni and concentrated solid solution alloys (CSAs, NiFe and NiCoCr) show a good agreement with the experimental results. We also conclude that the good agreement indicates the damage evolution under damage overlap conditions in Ni and CSAs at room temperature is dominated by defect recombination and migration induced by irradiation rather than activated thermally.

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