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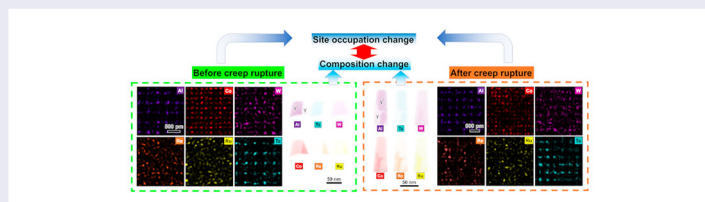
High-temperature creep-induced site occupation evolution in the γ' lattice in a Ru-bearing Ni-based superalloy

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ABSTRACT

By using state-of-the-art characterisation techniques including atom probe tomography and atomic resolved elemental mapping, we successfully probed the site occupation evolution associated with composition change in γ' , during 1100°C creep of a fourth generation Ru-bearing Ni-based superalloy. It is quantified that, W and Ru maintain unchanged site preference after creep rupture, while interestingly, the rest elements especially Co, Ta and Re show a weakened preference at both α - and β -sites in the γ' lattice. This indicates the overall reduced γ' ordering degree and thus the possible decrease in planar fault energies, which further facilitates dislocation shearing in γ' .



IMPACT STATEMENT

Associated with the tremendous mass transfer during high-temperature creep, the site-occupation scenario in the γ' lattice evolves as that, the preference at both α - and β -sites for Co, Ta and Re weakens while that of W and Ru remains nearly unchanged, indicating the overall decrease in ordering and thus the easier dislocation shearing in γ' .

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KEYWORDS

Ni-based superalloy;
Ru-bearing; site occupation;
ordering; creep rupture

1. Introduction

Ni-based superalloys, as a group of multicomponent and highly-concentrated alloy system, are known for their extraordinary temperature-capability even above 1000°C [1–6]. This is originated from a high-volume fraction of the strengthening γ' phase, which possesses the ordered $L1_2$ lattice containing distinctive face-center α and corner β sites [1,3,7–10]. Clearly, the site occupation behaviour among multiple alloying elements essentially determines the γ' nature, including the lattice parameter, modulus, friction stress and even the fault energies, which, affects the final strengthening effects.

Until now, many endeavours have been devoted to unravel the site occupation scenario. Starting from the

simple ternary Ni–Al–X alloys [11–15], it is well-known that Co substitute Ni at α -site while most other alloying elements e.g. Ti, Ta and Re substitute Al at β -site. However, in complex commercial systems with 5 or more principal elements, simulation methods are technically infeasible, and experimental strategies shall fit the requirements of high spatial and elemental resolution. Channelling enhanced microanalysis (ALCHEMI) [16–18] and atom probe tomography (APT) [19–22] have been applied, yet, it is argued that the accuracy of ALCHEMI remains questionable due to the complex experimental and data interpretation procedure, while that of APT relies on the appearance of a ‘pole’ artefact to locally enhance the spatial accuracy. Most recently, based

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on the probe-corrected transmission electron microscope (TEM), the atomic resolved energy dispersive spectroscopy (EDS) mapping endows the visualisation of the atoms (precisely, atom columns) even in multicomponent systems. Unfortunately, relevant reports are rare in Ni-base superalloys, and the existing few studies still leave the site occupation status of certain key elements e.g. Cr and Ru, into controversial [23,24].

When these superalloys are exposed to service conditions, e.g. creeping at high temperatures, rafting usually takes place, changing both the configurations and compositions of γ and γ' due to tremendous mass transfer [25–30]. This further renders the site occupation scenario more complex as it varies with the composition change, consequently triggering the evolution of the γ' nature. However, in Ni-based superalloys such atomic-scale microstructure evolution has long been ignored under service conditions, and its effect on the γ' strengthening behaviour is also unrevealed.

To address the concerns, in this work, we carried out a series of advanced characterisations on a fourth generation Ni-based superalloy, and carefully probed the site occupancy before and after creep rupture. It can be clearly seen that the site preference changes, in a way different from the partition behaviour between γ and γ' . Our findings will therefore contribute to a more thorough understanding on the elusive alloying effects of e.g. Re and Ru, in new-generation Ni-based superalloys.

2. Materials and methods

The nominal composition of the investigated Ni-based superalloy is Ni-23(Co + W + Mo)-2Cr-14(Al + Ta)-6Re-3Ru-0.2Hf-0.01C (all in wt.%), termed as 3Ru hereafter. The [001] single-crystal bar with a diameter of 15 mm was produced using a Bridgman furnace (ZGD-2) at a withdrawal rate of 4 mm/min. Samples were then subjected to a full heat-treatment sequence of 1325°C/4 h + 1330°C/6 h (air cooling, AC) + 1120°C/4 h (AC) + 870°C/24 h (AC). For the convenience of illustration we denote the full heat-treated state as the initial state.

The creep rupture experiment was carried out at a constant temperature/stress of 1100°C/140 MPa. After fracture (~ 300 h), samples for observation were taken about 5 mm away from the fracture surface to avoid excess plastic deformation and pores induced by necking. The sampling surface was kept normal to the stress direction, i.e. [001]. This sample state is then denoted as the ruptured state.

Overall microstructures (within the dendritic arm) were probed using a TEM (FEI Titan G2 60-300). Lattice parameters at room temperature were measured

using a high-resolution X-ray diffractometer (Bruker D8 DISCOVER). Precise composition was given via APT (Cameca LEAP 5000XR) under a laser pulsing mode with a pulse rate of 125 kHz and a pulse energy of 60 pJ. Atomic resolution elemental mapping was carried out on a double spherical aberration corrected TEM (FEI Spectra 300) equipped with a four-quadrant Super-X detector under the high-angle annular dark field (HAADF)-high resolution scanning TEM (HRSTEM) mode, with inner and outer semi-collection angles of 51 and 200 mrad, respectively. The collecting parameters include convergence angle 30 mrad, and probe current about 50 pA for HAADF-HRSTEM images and around 100 pA for EDS maps. A Radial Wiener filter was applied for the final EDS maps. TEM foils were prepared via twinjet electro-polishing in a solution consisting of 10% perchloric acid and 90% alcohol. APT tips were prepared via focus ion beam (FIB, FEI Helios Nanolab 600i) following a standard lift-out protocol.

3. Results and discussion

Figure 1(a) is the TEM bright field (BF) image showing the typical γ/γ' structure in the 3Ru-initial sample. The inset shows the selected range of X-ray diffraction pattern near the $[004]_{\gamma/\gamma'}$ peaks, where the γ/γ' lattice parameters and misfit is measured as 0.3643/0.3595 nm and -1.34% , respectively. This misfit value is relative large [31,32], directly leading to the fully cuboidal shape of the γ' phase and a high driving force to form misfit dislocation networks when rafting begins. Figure 1(b) shows the APT elemental distribution maps of Al, Co, W, Re, Ru and Ta. We distinguish Al and Ta (also Ni, not presented) as γ' -forming elements, Co, Re and Ru (also Cr and Mo, not presented) as γ -forming elements while W as with no partition tendency. The significant partition of Re and Ru to γ expands the γ lattice hence enlarges the negative lattice misfit between γ and γ' , in accordance to refs. [33–35]. Similarly, Figures 1(c) and (d) exhibit the TEM-BF image and the APT reconstruction maps of the 3Ru-ruptured sample. A typical N-type rafting architecture under the [001] zone axis appears, with dense dislocation networks filling up the γ/γ' interfaces [36,37]. As arrowed in Figure 1(c), only a few superdislocation pairs derived from the networks cut through the γ' rafts, confirming that the actual creep status at the sampled position was at the steady stage. In this state, the lattice parameters and misfit from the same (004) reflection (see the inset) are measured as 0.3606/0.3596 nm and -0.27% , respectively, much less negative as compared to that in the initial state. Although we failed to determine the (hk0) reflections to reflect the real γ/γ' misfit after rafting, the same trend, with a misfit value

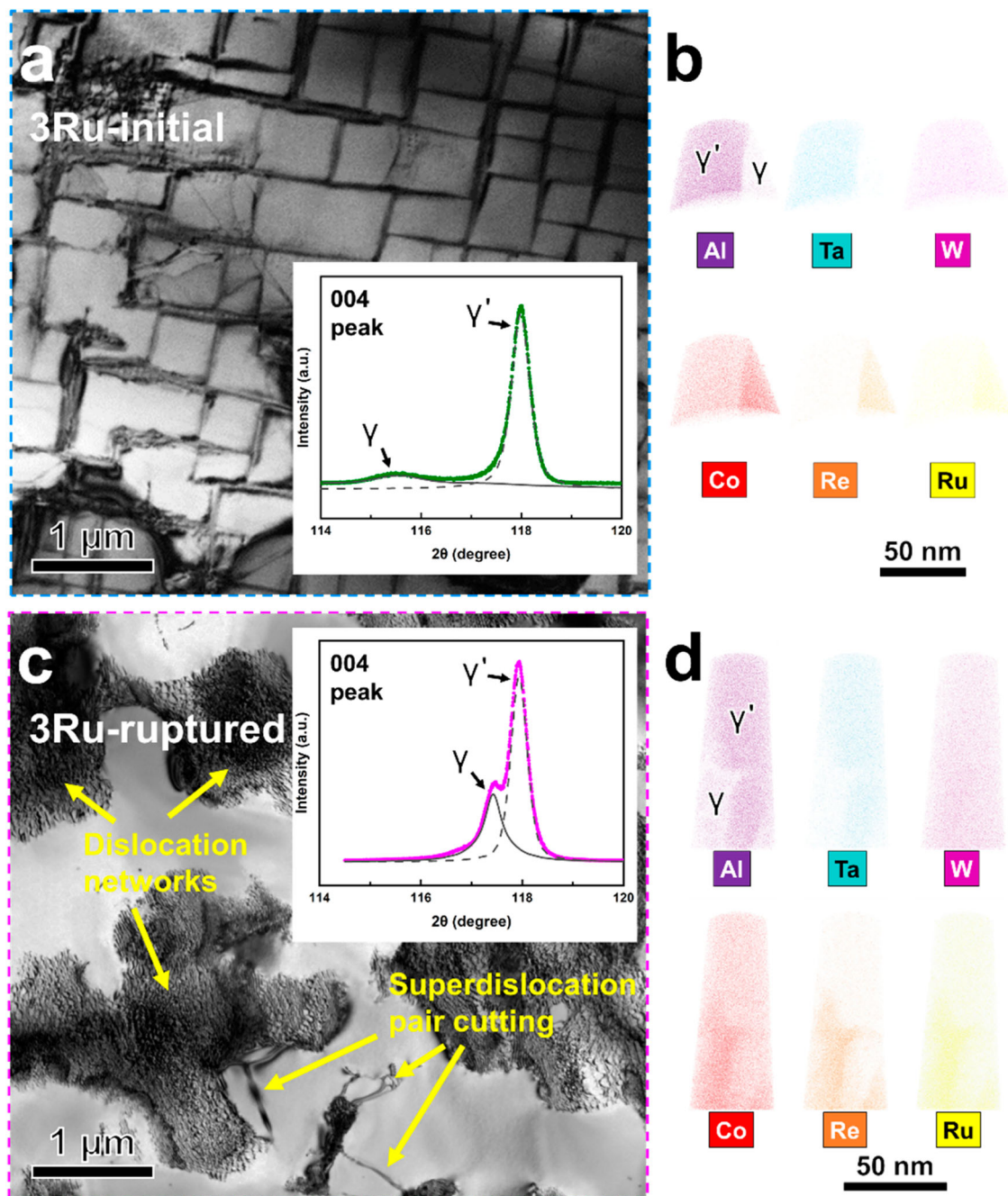


Figure 1. TEM bright field images and APT elemental maps (Al, Co, W, Re, Ru and Ta) of the 3Ru alloy at the initial (a, b) and ruptured (c, d) states, respectively. Notice that the X-ray diffraction patterns at each state are also included in the corresponding insets.

of -0.32% , is evidenced after the static annealing at the identical creep temperature and duration time, see Supplementary Materials, Figure S1. Such dramatic change in the absolute (001) misfit is also seen in the literature [37, 38, 39], indicating tremendous mass exchange between γ and γ' . Moreover, this may lower the interfacial dislocation density gradually during creep. To clarify this detailed investigation is required in the future. In Figure 1(d), similarly we observe both the γ and γ' phases with clear elemental partitioning, yet the γ/γ' interfaces are

much more curved as compared to those captured in Figure 1(b), agreeing well with the TEM result.

Figure 2 summarises the specific composition change of the γ' phase as well as the γ phase derived from the APT datasets. In γ' in Figure 2(a), amounts of γ' -forming elements Ni and Ta decline while that of Al arises. For γ -forming elements, Co, Re and Ru amounts increase the most, by 2.34 at.%, 0.17 at.% and 0.43 at.%, respectively. In γ in Figure 2(b), correspondingly, amounts of most γ' -forming elements increase while those of γ -forming

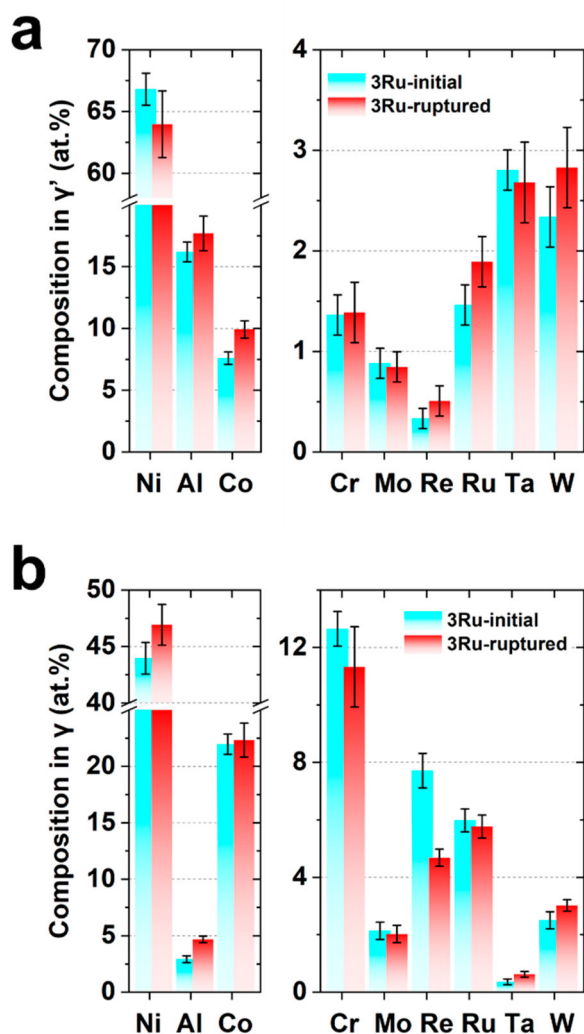


Figure 2. Composition change in (a) the γ' phase and (b) the γ phase between the initial state and the ruptured state of the 3Ru alloy, derived from the APT datasets shown in Figure 1.

elements decrease in different extends. Such flow of Re and Ru from γ to γ' and backwards of limit amount of Ta is therefore believed to be the main reason for the lattice misfit change. It is also noticed that the Ru concentration is almost fourfold of Re at both states (the multiple is usually 3~6 [33,40]). This suggests that although both are highly unfavoured in γ' , Ru is energetically more tolerable in the γ' lattice hence may play a more important role than Re in modulating the γ' nature especially during high-temperature servicing.

Figure 3 shows the atomic resolution EDS maps, where individual atom column under the [001] zone axis can be clearly distinguished (see the corresponding HAADF images in Supplementary Materials, Figure S12) and coloured based on the count intensity of each element. Since that each [001] atom column is either of pure α or of pure β as exemplified in the inset, a rough classification of the constitutional elements can be made out

of these maps. Ni and Co together belong to the first family that shows distinct α -site occupation. The second family includes Al, Ta and W that mainly stay at the β -site. The last family showing ambiguous tendencies involves the rest four elements, i.e. Re, Ru, Cr and Mo. This visual-based classification is too vague and a more quantitative landscape on the occupation tendency will be drawn next, considering two different ways.

In the first way, we resolve the variation of the count intensity linearly across several atom columns. Figures 4(a) and (b) show the Ni distribution maps representing the randomly selected array of atom columns along the $\langle 010 \rangle$ direction, and the corresponding intensity curves of e.g. Ta, W, Ru and Re, before and after rupture respectively. This column array contains alternate pure α - and β -sites as labelled, and we observe exactly the peak at the β -site while the bow at the α -site for Ta in both sample states. W behaves quite similarly yet weaker to Ta. Unfortunately, Re and Ru still show a much less significant variation between the two sites, and the difference between the two sample states remains inconspicuous. This is likely due to their low counts within the selected few atom columns, in a premise that they are both lean in the γ' phase (see Figure 2). To this end, we present the second way as statistically calculating the 'occupation coefficient'. In detail, we mark and count the numbers of all the pure α - (or pure β -) sites (which is fixed across all elemental distribution maps) and then count the number of such sites where the count of a certain element shows a maximum in the corresponding map. The occupation coefficient, hereafter denoted as δ , is then defined as the ratio of the two numbers (more details can be found in Supplementary Materials, Figure S3). Differing from the one defined in ref. [41], the term ' δ ' might not accurately determine the real site occupation, yet its value can reflect the tendency of elemental site occupancy statistically. The results are then listed and compared in Figures 4(c) and (d). In the α case in Figure 4(c), only Ni and Co show a $\delta\alpha$ over 0.5, while that of the rest elements remains below 0.2. This huge difference agrees well with the former discussion and thus, we reasonably set two threshold δ value, i.e. 0.5 and 0.2, where $\delta \geq 0.5$ means a strong tendency, $\delta \leq 0.2$ indicates barely no tendency, while when δ is in-between, it is considered the element showing a weak tendency to occupy this site. Notice that, although the value is still above 0.5, $\delta\alpha$ -Co sharply decreases after rupture, indicating that Co loses its overwhelming preference at the α -site. Turning to the β case in Figure 4(d), based on the proposed δ criterion we easily determine Al, Ta and W as the strong β -site preference elements. $\delta\beta$ -Ta drops profoundly after rupture, which also suggests the greatly weakened β -site preference for Ta. Elements Cr, Mo and Re present a similar weak tendency to occupy

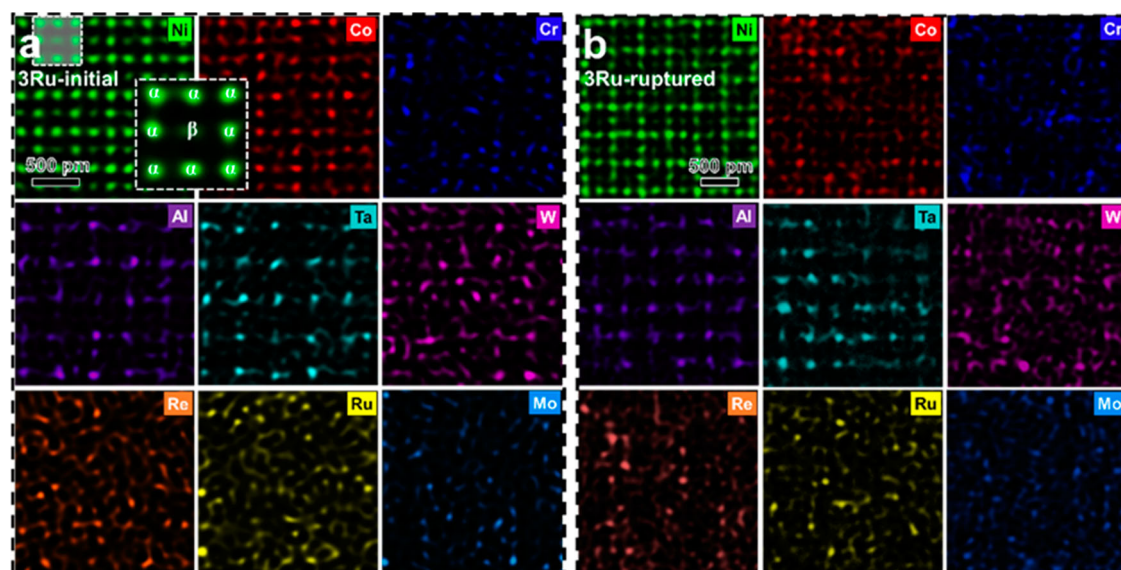


Figure 3. Atomic resolution EDS maps showing the elemental occupation at each atom column in the samples before (a) and after creep fracture (b). Notice that under the specific [001] zone axis these atom columns are either of pure α or of pure β as marked in the enlarged view in the inset.

β -site before rupture, where the performance of Cr supports the observation from refs. [12,23] but disagrees with those given in refs. [21,22,42]. After rupture however, their $\delta\beta$ values all decrease, and, $\delta\beta$ -Mo and $\delta\beta$ -Re are even down to 0.2, suggesting the vanishing of the initial weak β -site preference. For Ru, its $\delta\beta$ remains at around 0.2, hardly showing any β -site preference.

Considering together the above α and β cases, we find that firstly, no element shows high $\delta\alpha$ and $\delta\beta$ simultaneously, confirming the proposed parameter δ being self-consistent. Secondly, during high-temperature creep, the core α -site element Ni and core β -site element Al, each keeps the highest δ at ~ 1.0 for α and β , respectively. This is reasonable since the γ' lattice will energetically maintain the Ni₃-Al framework unless approaching its dissolution temperature. Thirdly, after creep W and Ru show nearly unchanged δ . W is well-known for its rather weak γ/γ' partition tendency in Ni-based superalloys [43,44], which is also confirmed in our APT results. The steady W flow between γ and γ' with slight amount increase in γ' likely helps with its unchanged δ level since W behaves like insensitive to the chemical environment change and probably shows a steady bounding to the core elements Ni and Al in the Ni₃Al-type γ' lattice. Ru is usually believed to show β -site preference, either through simulation or by ALCHEMI in simple alloy systems [11,13,15–17,45]. However, recently in an experimental study on another commercial Ni-based superalloy [23], Ru is proposed to oppositely exhibit the α -site preference, which agrees with a simulation result [46]. This is attributed to the similar d-band filling state of

Ru to Co, leading to a comparable α -site occupation tendency [47]. From these competing results, it is induced that Ru might not show occupation preference at either site, and its site occupancy can vary with the specific chemical environment and temperature as mentioned by Jiang et al. [48]. Our measurements also support this statement and at least in the investigated Ni-based superalloy, Re shows a stronger β -site preference than Ru at the initial state, even the concentration in γ' is much lower than Ru.

Intriguingly besides Ni, Al, W and Ru, all the rest elements show a decreasing tendency of δ after creep rupture, whether at α - or β -site. This indicates that the overall site preference is weakened. We suppose that this is a sign of disordering of the γ' -L1₂ structure, which seems reasonable after creep at high temperatures, i.e. 1100 °C here [49]. According to the classical Gibbs free energy equation: $G = \Delta H - T \cdot \Delta S$, the increased environmental temperature T enlarges the entropy effect (ΔS), which further lowers the system free energy towards the full-solid-solution hence reduces the ordering degree. Apparently, this results in the so-called thermal equilibrium effect. Creep-induced dislocations also play a role in the thermodynamic disordering process via the following two ways. Firstly, the dense interfacial dislocation networks act as fast diffusion paths, accelerating mass flow needed for disordering. And secondly, the sweeping of the observed superdislocations across the γ' lattice creates fault structures and even triggers local phase transformation, destroying the ordered atomic stacking and consequently, contributing minorly to the reduced

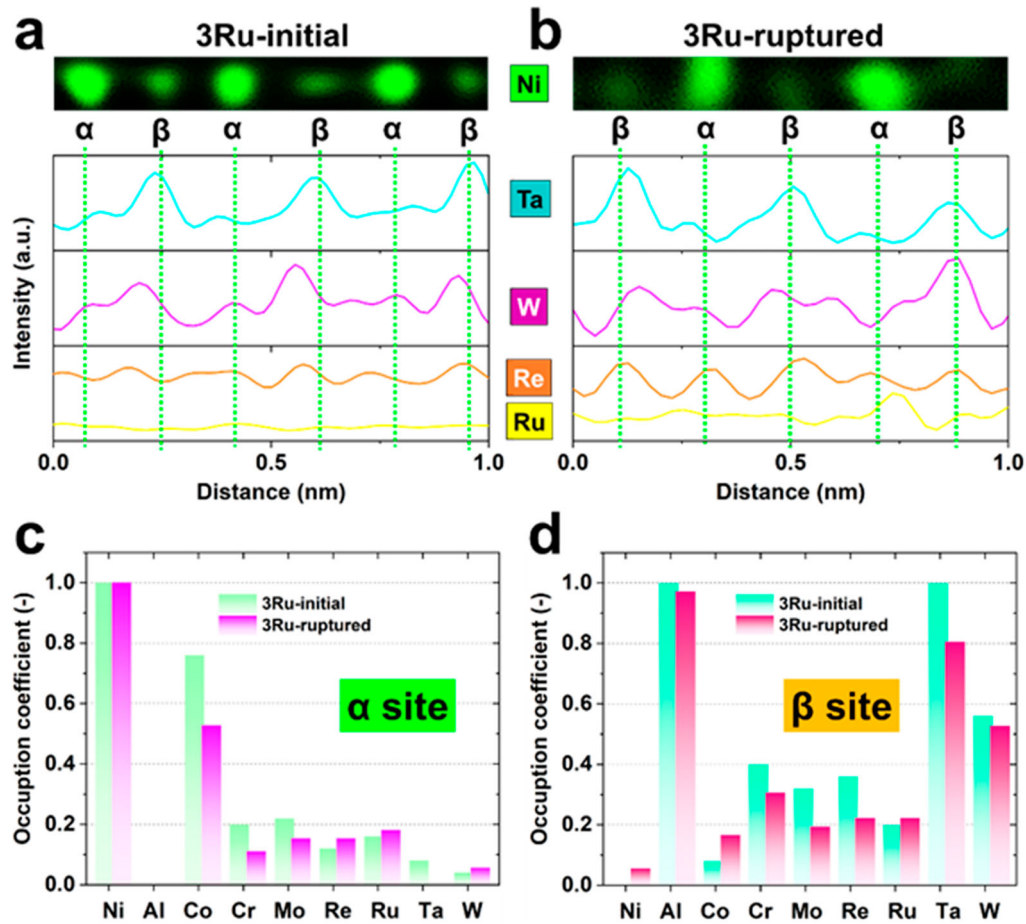


Figure 4. Variation of the count intensity linearly across several atom columns along the $\langle 010 \rangle$ orientation, (a) for the initial state and (b) for the ruptured state, taken Ta, W, Re and Ru for example. Calculated occupation coefficient δ of each constituent element at (c) α - and (d) β -site.

ordering degree [50–53]. The occurrence of disordering, firstly, lowers the stability of γ' and in turn triggers the re-establishment of the phase equilibrium at such high temperature [30]. As a result, the γ' fraction decreases, and thus the strengthening effect loses. Secondly, the absolute lattice misfit decreases (as evidenced in Figure 1) associating with re-establishing phase equilibrium, which probably leads to the in-situ decrease in interfacial dislocation density and thus the decrease in shearing resistance of the channel dislocations. At last and more importantly, it reduces the fault energies of γ' (e.g. anti-phase boundary energy and stacking fault energy) that are closely related to the ordering status and alloying status as well [53–55], promoting the formation of those fault-related structures within the γ' rafts. This will accelerate and multiply dislocation shearing events that leads to breakdown of the rafts, shortening the steady-state creep duration thereby detrimental to the creep performance.

4. Conclusion

In this study, by using the state-of-the-art atomic-scale characterisation techniques including APT and double spherical aberration corrected TEM, we successfully probed the lattice misfit, the composition change in γ' and the associated evolution of the α/β site occupation with the aid of a statistical parameter δ , after 1100°C creep rupture. It is found that large amount of γ -forming elements including Co, Cr and in particular Re and Ru flow into γ' , leading to the sharply reduced γ/γ' lattice misfit. Upon such mass flow, W remains with nearly unchanged strong β -site preference and Ru shows no obvious site preference. It is intriguingly to point out that, all the rest elements, including Co, Re and even Ta, show a weakened site preference at both α - and β -sites. This is due to the overall reduced ordering degree of γ' during high-temperature creep, which likely reduces the fault energies hence facilitates multiple shearing events within the γ' rafts.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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Data availability

The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of other ongoing studies.

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