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# Temperature dependence of strengthening mechanisms in the nanostructured ferritic alloy 14YWT: Part II—Mechanistic models and predictions

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ABSTRACT

The temperature dependence of strengthening mechanisms in the nanocluster-strengthened 14YWT alloy was investigated to elucidate the relative significance of contributing mechanisms in different temperature ranges. This study was also aimed at providing the prediction capability of yield strength for the nanostructured ferritic alloys over a wide range of temperature. The four major strengthening mechanisms: the Peierls stress, grain boundary strengthening, direct nanocluster strengthening, and dislocation forest hardening, were taken into account in the calculation, and their roles and characteristics in different temperature ranges were extensively discussed. The results indicated that the contribution of grain boundary strengthening to total strengthening was the most significant component. Yield strength calculation was made by combining all the strengthening components and the results were compared with the experimental data. Further, the validation of the proposed approach was attempted by applying to the yield strength of other alloys.



## 1. Introduction

The present paper (Part II) is a sequel to the previous paper (Part I) dealing with mechanical properties and microstructural observations for nanostructured ferritic alloys (NFAs), which are well known for their excellent high temperature strength and resistance to irradiation damage due to the presence of uniformly dispersed nanoclusters (NCs) [1–5]. Although the excellent high temperature strength leads to a high creep resistance which is key property for future high temperature reactor applications, it is believed to be obtained at the expense of ductility and toughness. It is needed therefore that the yield strength (YS) of the alloys is controlled to have an optimized combination of strength, ductility, and other mechanical properties.

Although understanding strengthening mechanisms in the NFAs is essential for the property optimization, the explanation for what strengthening effects (NCs, high dislocation density, solid solution, grain boundary strengthening, etc.) contribute to the YS at what temperature regime has not been clearly made. The NCs have been thought to be a major source of the strong strengthening but the lattice friction, grain boundary strengthening, and high dislocation density are also important strengthening sources. It should be possible to evaluate contributions by these mechanisms if sufficient information on the microstructure coupled with rigorous physical models is utilized [6]. The main goals of this study are to evaluate the roles of individual hardening mechanisms over a wide range of temperature and to facilitate an integrated mechanistic model for future uses for NFAs.

The summation of the strengthening components can be categorized into three temperature regimes as shown in Fig. 4 of Part I. Therefore, it is necessary to discuss the strengthening mechanism with respect to temperature ranges, *i.e.* very low temperatures, ambient temperatures, and high temperatures. With respect to these temperature ranges, dominant mechanisms and related formulations are described here. In Part I, mechanical properties and microstructural observations for the nonirradiated 14YWT steel [7,8] were discussed. In this part, the YS prediction models were studied on the basis of the microstructural parameters observed in Part I.

## 2. Estimation of temperature dependence of yield strength

### 2.1. Strengthening mechanisms between room temperature and 600 °C

It is well granted that the resistance of obstacles to dislocation glide determines the flow stress of alloys. Since the NFAs consist

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of numerous NCs, nanograin boundaries, dislocations, precipitations etc., it is expected that many different types of obstacles affect dislocation motion. Also, secondary contributions should exist through interactions in the forms of line tension of bowed-out dislocations, and cutting or by-passing of NCs [9,10]. In the present work, the increase of YS is approximately expressed by four strengthening components: grain boundary strengthening ($\Delta\sigma_k$), direct strengthening of NCs ($\Delta\sigma_p$), dislocation forest hardening ($\Delta\sigma_\rho$), and matrix hardening ($\Delta\sigma_m$). The details of respective component are discussed below.

#### 2.1.1. Direct strengthening of nanoclusters ($\Delta\sigma_p$)

Deriving an expression for the strengthening component by NCs requires significant postulates since the nature of their interaction with dislocations is not well understood. Previous works suggested an Orowan by-pass mechanism in nanostructured ferritic or ferritic/martensitic alloys [11–14]. Assuming that NCs are impenetrable incoherent particles, the direct NC strengthening due to Orowan dislocation by-pass can be described by Eq. (1) [15],

$$\Delta\sigma_{or} = \frac{0.81MGb}{2\pi(1-\nu)^{1/2}} \frac{\ln(2r_s/r_0)}{\lambda-2r_s}, \quad (1)$$

where $M$ is the Taylor factor, $G$ the shear modulus ($=93.2\times(1-4.368\times10^{-4}T\,\text{GPa})$), $b$ the magnitude of the Burgers vector, $\lambda$ the mean planar center to the center distance between NCs, $r_0$ the inner cut-off radius of a dislocation core, which is assumed to be the magnitude of the Burgers vector, and $r_s=0.816\times r$ is the mean planar particle radius of the cross-section of a particle of radius $r$. In this approach, the most sensitive parameters are $r$ and the number density of NCs. From literature survey and observation in the first part of present paper, they are determined as 1.9–2.1 nm and $(1–5)\times10^{23}\,\text{m}^{-3}$, respectively [16–18]. However, since the NCs located at grain boundaries may not interact directly with moving dislocations inside grains, present approach used the information on the NCs located at grain interior, i.e. $r$ of $\sim$1.9 nm and number density of $(0.8–4)\times10^{23}\,\text{m}^{-3}$. Determination of $\lambda$ was done on the basis of a random array of obstacles [15] using the following expression [19]:

$$\lambda = 2\sqrt{\frac{2}{3}}r\left[\left(\frac{\pi}{4f}\right)^{1/2}-1\right], \quad (2)$$

where $f$ is the volume fraction of NCs. It is noted that the calculated $\lambda$ value is quite sensitive to the number density of NCs, and therefore the uncertainty in the number density information can bring about a considerable amount of error in the particle strengthening prediction. On the other hand, the interaction of dislocations with the coarse oxide particles was neglected since Eq. (1) yields $\sigma_{or}<50$ MPa for oxide particles $>100$ nm in size.

Seeger [20] introduced another approach: the dispersed barrier hardening model which is based on straightforward geometrical considerations for obstacles intersecting the dislocation glide plane [21];

$$\Delta\sigma_{dbh} = 0.8M\alpha(r)Gb/\lambda, \quad (3)$$

where $\alpha(r)$ is a barrier strength coefficient representing the strength of defect clusters as obstacles to dislocation motion. In principle, the barrier strength coefficient is determined by the angle between adjacent dislocation segments at the point where the dislocation breaks free of the obstacle [22]; if the critical angle is $\varphi$, the barrier strength coefficient equals to $\cos(\varphi/2)$. Alinger [6] found that $\alpha(r)$ increases approximately linearly with $\log(r/2b)$ by fitting the coefficient to experimental dataset of several NFAs and proposed the function of $\alpha(r)$ as shown below,

$$\alpha(r) = -0.017+0.374\log(r/2b). \quad (4)$$

It was reported that the barrier strengths for the visible defect clusters in neutron irradiated V–4Cr–4Ti [23] and other BCC metals [24] are 0.4 or higher. When the barriers are impenetrable, then $\alpha(r)=1$ and this is the case for Orowan by-pass mechanism. In the present work, $\alpha(r)$ is calculated as $\sim$0.20 whereas a range of $\alpha(r)$ between approximately 0.05 and 0.30 indicates that the small NCs are relatively soft obstacles, either because they can be sheared by dislocations or because of dipole interactions between highly bowed dislocation segments [25].

This hypothesis is reasonable because the nanometer-scale clusters would not be strong enough to produce bowing angles of $\approx0^\circ$. Also, this assumption is supported by the present TEM observations with no clear observation of Orowan loops around NCs.

The magnitude of the direct strengthening due to NCs in both approaches is summarized in Table 1 as a function of temperature. In these approaches, the shear modulus, $G$, is the only parameter that is temperature dependent. It is noted that the direct strengthening on the basis of the dispersed-barrier-hardening model is around one third of the conventional Orowan by-pass model. Also, it is noted that the calculation of direct strengthening is very sensitive to the number density of NCs ($8\times10^{22}\,\text{m}^{-3}$–$4\times10^{23}\,\text{m}^{-3}$). However, it is very difficult to measure the number density precisely within an error range of 10% and the results differ for different measurement methods. Moreover, the distribution of NCs is not perfectly homogeneous throughout the microstructure. Thus, the second best approach is to make both cases upper and lower limits, respectively, and then compare with the experimental results.

#### 2.1.2. Hall–Petch strengthening

It is well known that the grain boundary strengthening is very important in ultra-fine grained materials. In particular, the present alloy has very fine grain size of $\sim$160 nm. Recently,

**Table 1**
The amount of direct strengthening due to NCs calculated basis on Orowan by-passing or dispersed-barrier-hardening model. $n$ means the number of NCs per $\text{m}^3$.

| Temperature (°C) | Orowan hardening (MPa) | | Dispersed-barrier-hardening (MPa) | |
|---|---|---|---|---|
| | $n=8\times10^{22}\,\text{m}^{-3}$ | $n=4\times10^{23}\,\text{m}^{-3}$ | $n=8\times10^{22}\,\text{m}^{-3}$ | $n=4\times10^{23}\,\text{m}^{-3}$ |
| 25 | 468 | 1196 | 178 | 417 |
| 200 | 432 | 1106 | 164 | 386 |
| 300 | 408 | 1045 | 155 | 364 |
| 400 | 385 | 984 | 146 | 343 |
| 500 | 361 | 923 | 137 | 322 |
| 600 | 337 | 862 | 128 | 301 |
| 700 | 313 | 801 | 119 | 279 |
| 800 | 290 | 741 | 110 | 258 |
| 900 | 266 | 680 | 101 | 237 |
| 1000 | 242 | 619 | 92 | 216 |