Relation between Yield Stress and Peierls Stress

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Abstract

It is often assumed that the Peierls stress of single dislocations can reflect accurately the macroscopic yield stress. Here, dislocation dynamics simulations show that the yield stress-to-Peierls stress (Y/P) ratio remains in a small range of ~ 0.3 ± 0.1, over a wide range of initial dislocation density, mobile dislocation fraction, and temperature which affects cross slip. This range of Y/P arises from the typical stress concentration ahead of dislocation pile-ups. The results explain why Y/P was observed to be around one-third in previous experiments.

Keywords: Dislocation; yielding; Peierls stress; back stress; dislocation dynamics simulation

Understanding the nature of plastic deformation of crystalline metals has been an important topic since the earliest days of physical metallurgy. Upon the application of increasing stress crystalline metals undergo a transition from elastic deformation to plastic flow by collective dislocation motion, which is known as yielding. Yielding is usually viewed as a smooth and steady flow on macroscopic scales. However, in recent decades a new picture has emerged [1, 2], namely, yielding is seen as a result of group interactive behavior of dislocations. It is also well known that plastic deformation is characterized by intermittent strain bursts which are also known as dislocation avalanches [3]. When plastic deformation is occurring in micron-scale crystals, internal dislocation avalanches lead to power-law like distributions of strain bursts [4], while macroscopically yielding may appear as a smooth process due to the large number of randomly oriented crystals involved.

Dislocation avalanches depend on the movement and multiplication of dislocations, which are constrained by the Peierls stress. Even though Peierls stress is widely regarded as the most important factor controlling plastic yield, how Peierls stress is related to yield stress is still not well understood. The literature is full of the assumption that the Peierls stress equals the critical resolved shear stress (CRSS) for high-purity single crystals while for bulk samples the value is obtained by extrapolating the CRSS to 0 K (e.g. [5, 6]), but this assumption has never been confirmed, and in fact, by some basic reasoning, it can be envisaged that it is not correct. For instance, it has already become well known that when there is no or insufficient dislocations in the crystal (e.g. the case of nano-cyrstals), the yield stress would approach the theoretical strength limit due to the lack of carriers for deformation. Another possible situation is that when the dislocation density is very high, mutual interactions of dislocations can affect their effective glide stress and movement, and thus the yield stress.

In fact, studies in the past have shown that the yield stress can be significantly lower than the Peierls stress. The ratio between yield stress and Peierls stress (Y/P) was found to be roughly 1/3 over a wide range of temperatures in both experiments [7, 8] and simulations [9, 10]. It has been conjectured that a systematic stress concentration inside the deforming crystal increases the true stress experienced by a typical traversing dislocation to significantly above overall applied stress [7, 8]. The origin of such stress concentration is akin to the avalanche effect which produces sudden yield or strain bursts [11].

Besides Peierls stress and the presence of other dislocations, another factor can affect dislocation pile-ups and avalanches. In a recent study of partitioned steel which has both high strength and ductility [12], the ductility of the steel is explained by the presence of mobile dislocations. In that study about 20% of mobile dislocations were estimated [12]. It was also conjectured that when the applied stress is high enough, the mobile dislocations unlock the immobile dislocations (the remaining ~80% of the dislocations) and trigger an avalanche and result in ductility.

Given the above background, this study aims at gaining insights into under what conditions will the yield stress be significantly smaller than the Peierls stress. Two-dimensional dislocation dynamics (DD) simulations were employed to investigate the relation between the Y/P ratio, dislocation density and percentage of mobile dislocations.

The DD model used here is similar to that used in a previous study [13], and so only the key concepts are described. The simulation region is a square with side length of 2000 Burgers vectors. Initially different densities (10^{12}, 10^{13}, 10^{14}, 10^{15} and 10^{16} m^{-2}) of parallel, screw dislocations with randomly assigned signs and positions are allocated in two mutually perpendicular glide planes. The applied shear stress acts on a plane at 45^o to both slip planes so as to produce equal resolved stress on them. Periodic boundary condition is applied to the four boundaries. Specific features of the simulations are as follows:

Peierls barriers and mobile dislocations – Dislocation avalanches are due to the sudden release of dislocations which are initially captured at barriers (referred to here as the Peierls barriers in general), and in a deforming crystal, it is likely that not all dislocations are initially locked. In order to simulate the group interactive behavior of dislocations, a certain fraction of dislocations are given a specific Peierls stress value according to the Peierls-Nabarro model: $\tau_p = \frac{2\mu}{1-\nu} exp\left(\frac{-2\pi w}{b}\right)$ [14, 15], while the remaining dislocations are assumed mobile with a much lower resistance stress of 1% of τ_p. Different fractions (from 0 to 100%) of the mobile dislocations were used to see the effects on the strength and strain achieved. Once an initially locked dislocation is unlocked, the lattice resistance is decreased to 1% of τ_p since it has become mobile.

Dynamics – Under an externally applied stress τ_{app}, the total glide stress on the dislocations is $\tau_{total} = \tau_{app} + \tau_{int} - c\tau_p - \tau_{obs}$. Here c is 1 or 0.01 according to whether the dislocation is locked or mobile, and τ_{int} is the pair-wise elastic interaction stress between dislocations given by $\mu b_i b_j /(2\pi r_{ij})$, where μ is the shear modulus, b_i and b_j are the Burgers vectors of the interacting pair, and r_{ij} is their distance. τ_{obs} is the resistance from obstacles such as precipitates, for simplicity it is assumed zero in this study. The glide force is calculated as the component of the total force on the glide plane, and dislocation velocity is assumed to obey a law: $v = v_o(\tau_{total}/\tau_o)$, where τ_o and v_o are constants. Annihilation of dislocations occurs whenever two opposite signed dislocations come to a distance shorter than $1b$. Load is applied at a constant rate of 2MPa/s, and the proof strength at 0.05% strain is determined to represent the yield stress Y.

Cross slip and temperature effects – Dislocations are allowed to cross slip onto another slip plane, when the cross-slip force (the component of the total force on the cross-slip plane) is large enough. For the results presented in Figs. 1 to 3 below, cross slip is allowed to occur with a 5% probability when the ratio of the cross-slip force to the glide force exceeds 5. In a set of simulations shown in Fig. 4, the thermal effect on cross slip is studied. Here, the cross slip probability *P* takes the form $P = \chi \exp\left[-V\frac{\tau_{III}-\tau}{kT}\right]$, following ref. [16, 17]. The factor χ is set as 5, V is set at $300b^3$ according to Groh et al. [16]. τ is set to be 5 times of the glide plane stress at the onset of yielding in the simulation. The τ_{III} value is chosen to be 1053 MPa [18], which is the CRSS at the onset of stage-III hardening for steel.

Fig. 1 shows the Y/P ratio for different fractions of mobile dislocations and dislocation densities. It can be seen that if the percentage of mobile dislocations is very low, the external applied stress must be close to the Peierls stress in order to trigger yielding. As the percentage of mobile dislocations increases, there is a general decrease of the yield stress relative to the Peierls stress, and it is obvious that the presence of more mobile dislocations makes yielding easier. However, it is interesting to see that a small increase in mobile dislocations from 0 to ~ 20% causes a rapid drop in the yield stress up, and beyond ~20% of mobile dislocations, the yield stress would not drop much further, and the Y/P ratio falls in the range of ~ 0.3 ± 0.1 for the different initial dislocation densities simulated. It is also observed that a higher initial dislocation density favors the lowering of yield stress. With a lower dislocation density such as 10^{12} m^{-2}, even when all dislocations are mobile and experience the low friction stress of 0.01 P, the Y/P ratio can barely drop to below ~ 1/3, but for a higher dislocation density such as 10^{16} m^{-2}, around 20% of mobile dislocations is enough to cause the Y/P ratio to drop to 1/3.

In the present simulations, those dislocations initially locked by the Peierls stress produce pile-ups behind them, and the stress acting on the leading dislocation would be magnified due to the stress concentration effect of the trailing dislocations. Fig. 2 shows how stress concentration unlocks a dislocation with high Peierls stress. The inset of Fig. 2 shows a locked dislocation (red dot) behind which a few of other dislocations (blue dots) pile up. As the mobile dislocations pile up against the locked dislocation, the accumulated stress becomes large enough to overcome the Peierls stress, and then the leading dislocation becomes unlocked and moves. The main panel in Fig. 2 shows the probability density of the stress concentration factor from the collection of locked dislocations in the system with initial dislocation density of 10^{16} m^{-2} just before yielding occurs. The stress concentration factor here is the ratio of the effective stress (i.e. total stress on the dislocation not counting the Peierls stress) to the applied stress. It can the seen that the stress concentration factor peaks at around 2 to 4, meaning that just before yielding, most locked dislocations experience a stress 2 to 4 times of the applied stress due to the stress concentration effect of pile-ups. Exceptions are found in the cases of 0% and 100% of mobile dislocations, where all the dislocations in the system have the same resistance stress (of P and 0.01 P respectively), so that no dislocation is statistically different than others and thus the stress concentration effect disappears (modal stress concentration factor becomes 1). The occurrence of a peak in all the other cases indicates that the majority of locked dislocation are experiencing similar level of stress. At this point the effective stress is about the same as the Peierls stress, and yielding with noticeable strain soon follows. The reciprocal of the modal stress concentration factors of about 2 to 4 here fall in the range of ~ 0.25 to 0.5, which agrees quite well with the typical Y/P ratio of ~ 0.3 ± 0.1 in Fig. 1. The Y/P ratio is evidently a stress concentration effect of dislocation pile ups in the system.

Fig. 3 further illustrates how much stress is needed to trigger a dislocation avalanche when the dislocation density is 10^{16} m^{-2}. In this case the percentage of moving dislocations is counted for different stress levels with different percentages of mobile dislocations. Here, moving dislocations are those with non-zero velocities, while mobile dislocations simply mean those dislocations that are initially assigned the lower resistance of $0.01\tau_p$. Therefore, a mobile dislocation will not be actually moving if the glide force on it is zero, and once an initially locked dislocation is unlocked, it is counted as moving. A rapid rise in the fraction of moving dislocations therefore indicates an avalanche, as a large number of initially stationary dislocations are set into motion. Fig. 3 shows that if there is no mobile dislocation to start with, the applied stress must be close to the Peierls stress in order to trigger an avalanche. But for 20% or higher mobile dislocations, the sharp increase of moving dislocations and thus avalanche occurs at applied stress around 0.15 to 0.3 times of the Peierls stress, implying that only 15 to 30% of the Peierls stress is needed to trigger dislocation avalanche and yielding.

The results in Figs. 1 and 3 clearly indicate the condition for avalanche and yielding to occur, which matches experimental observations. As mentioned above, the ratio between yield stress and Peierls stress (Y/P ratio) is roughly 1/3 in experiments [7]. In the present simulations, this is the case for a wide range of dislocation density and fraction of mobile dislocations. Also, the present results also explain why a relatively small amount of mobile dislocations (20%) can trigger dislocations avalanches and induce ductility in some metals [12]. To simulate the effects of temperature, thermal assistance of cross slip is modeled by a temperature-dependent cross-slip probability as described above. Fig. 4 shows the Y/P ratio for temperature ranging from 50 to 400K, for the case of 10^{16} m^{-2} initial dislocation density and 20% of mobile dislocations. It can be seen that for a wide range of temperature the Y/P ratio is between 0.25 to 0.35, which is very close to the experimental value of 0.3 to 0.4 [7].

In this study, a dislocation initially trapped in a Peierls barrier is reassigned a much reduced lattice friction once it starts moving, which is a mechanism related to the yield-point phenomenon [19]. The results in this study therefore provide the insight that similar mechanisms might have occurred in the experimental studies in ref. [7, 8, 12] for ferritic iron or partitioned steel. The present results also show that both the fraction of mobile dislocations and the dislocation density control the yielding of metals. In a recent study of a novel partitioned steel [12] with unprecedented high strength and ductility, a high dislocation density led to high strength due to Taylor hardening, and the authors estimated that about 20% of the dislocations were less trapped by solutes or precipitates and were therefore mobile. They further conjectured that, when the applied stress was not high enough, the mobile dislocations could not unlock the remaining ~80% of dislocations which were immobile so that yield would not occur, but when the applied stress was high enough, the mobile dislocations would trigger an avalanche and then the material would suddenly yield with some ductility. The present simulations confirm this picture of group effects of dislocations, namely, when the mobile dislocation fraction is about 20%, dislocation avalanche and thus yield can be produced by an applied stress about 1/3 of the locking stress of the initially immobile dislocations. In general, depending on the dislocation density and fraction of mobile dislocations, significant micro-slip processes can take place even when the applied stress is significantly lower than the Peierls stress, and the usual assumption that the locking stress of immobile dislocations reflects the yield stress may not be valid.

To conclude, the present simulations show that at an applied stress of around 0.3 ± 0.1 of the Peierls stress, the presence of ~20% of mobile dislocations can trigger an avalanche of the remaining ~80% of dislocations which are initially locked by Peierls barriers, leading to yielding. The Y/P ratio of 0.3 ± 0.1 is found to be valid for a wide range of initial dislocation density, and matches previous experimental results.

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Figure Captions

Fig. 1. Contour plot of Y/P ratio against dislocation densities and percentage of mobile dislocations.

Fig. 2. Stress concentration in dislocation pile-ups. Inset shows formation of a dislocation pile-up against an initially locked dislocation, leading to the release of the dislocation as the stress builds up. Main panel shows probability density of the stress concentration factor (ratio of total stress on the dislocation not counting the Peierls stress, to the applied stress) for all the locked dislocations in the system just before yielding, in the simulation case of dislocation density of 10^{16} m^{-2} with different percentages of mobile dislocations.

Fig. 3. The percentage of moving dislocations vs different ratios of applied stress to Peierls stress, with different percentage of mobile dislocations. Initial dislocation density is 10^{16} m^{-2}.

Fig. 4. Y/P ratio for temperature ranging from 50 to 400K for 10^{16} m^{-2} dislocation density of which 20% is mobile.

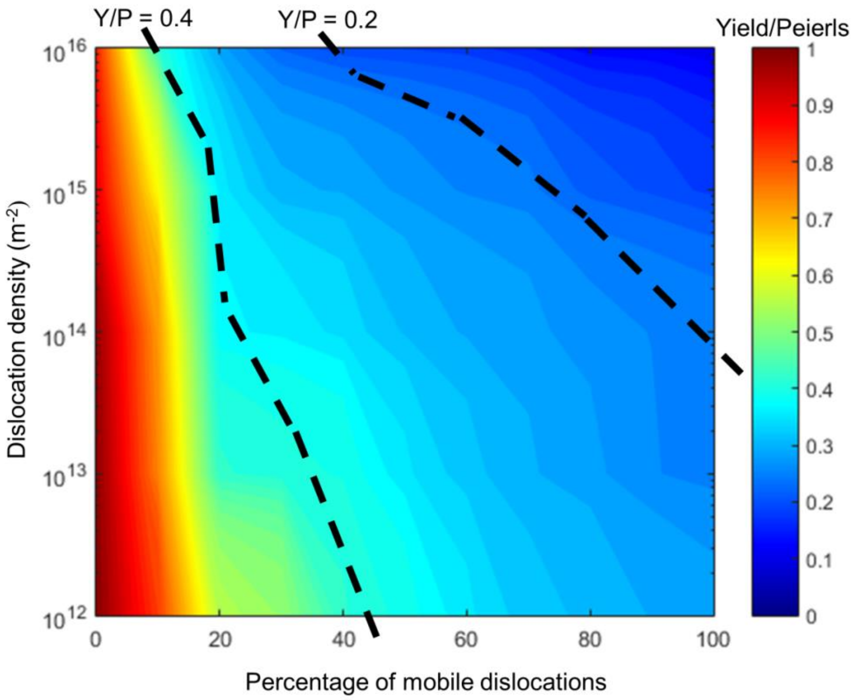
Y/P = 0.4
Y/P = 0.2
Yield/Peierls
Dislocation density (m-2)
Percentage of mobile dislocations

Fig. 1

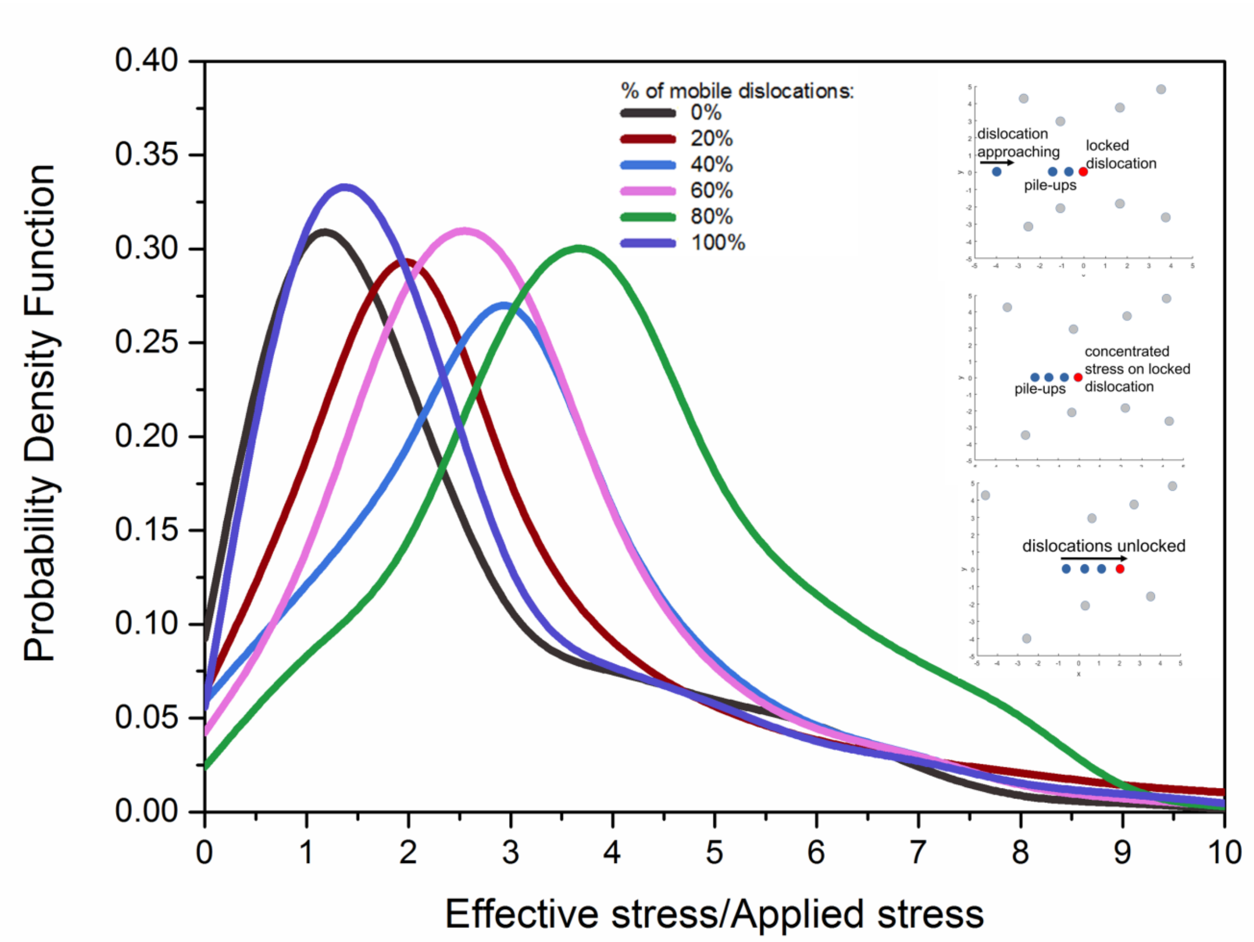
Probability Density Function
Effective stress/Applied stress
% of mobile dislocations:
0%
20%
40%
60%
80%
100%
dislocation approaching
locked dislocation
pile-ups
concentrated stress on locked dislocation
pile-ups
dislocations unlocked

Fig. 2

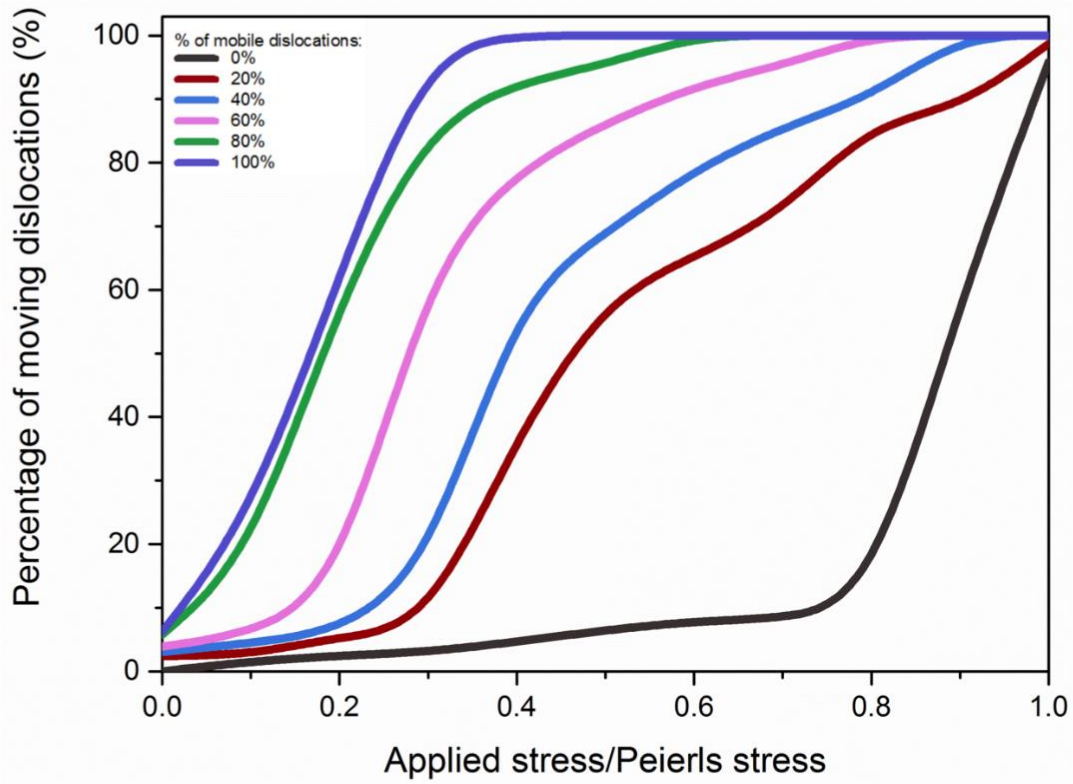
Percentage of moving dislocations (%)
% of mobile dislocations:
0%
20%
40%
60%
80%
100%
100
80
60
40
20
0
0.0
0.2
0.4
0.6
0.8
1.0
Applied stress/Peierls stress

Fig. 3

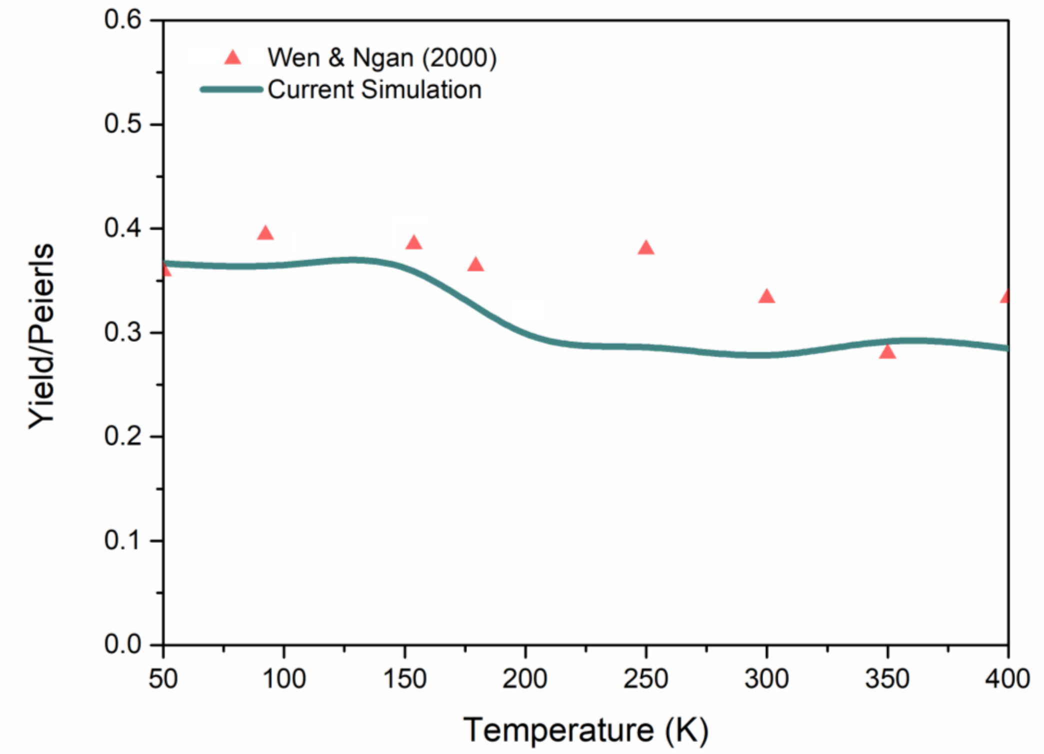
Wen & Ngan (2000)
Current Simulation
Yield/Peierls
0.6
0.5
0.4
0.3
0.2
0.1
0.0
50
100
150
200
250
300
350
400
Temperature (K)

Fig. 4

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