

The plastic deformation of potassium single crystals at low temperatures

G. S. MURTY

Department of Metallurgical Engineering, Indian Institute of Technology, Kanpur, India

The yield stress of potassium single crystals was measured in the temperature range of 1.5 to 30 K for a wide range of orientations. The effects of substitutional solutes (sodium and rubidium) on the yield strength of potassium single crystals were also investigated. The Schmid law of critical resolved shear stress for slip is invalid in the temperature-dependent region of yield stress, and the orientation dependence of yield stress is in agreement with the Peierls mechanism for screw dislocation motion. The validity of the Schmid law may be questionable even in the athermal region, as suggested by the observations at 30 K. Alloy softening is observed in the temperature-dependent region of yield stress by adding substitutional solutes to potassium.

1. Introduction

There are several striking features in the plastic behaviour of the body centred cubic (bcc) metals. The yield stress of bcc metals is strongly temperature-dependent, with the thermal component being several times larger than the athermal component in the very low temperature regime. The slip geometry in bcc metals is complex and the Schmid law of critical resolved shear stress (CRSS) for slip breaks down at low temperatures. While the slip direction is $\langle 111 \rangle$, the operative slip plane differs widely depending on temperature, orientation of the crystal, sense of the applied stress, the species of metal and its purity. Several planes of nearly equal density of packing, $\{110\}$, $\{112\}$ and $\{123\}$, and a maximum resolved shear stress plane (MRSSP) belonging to the zone of slip direction have been identified as operating slip planes in different bcc metals under various conditions. While the slip lines tend to be straight at all points of the intersection of the glide zone with crystal surface at the very low test temperature, these are wavy in the higher temperature range except when the surface is nearly parallel to the slip direction. Several reviews [1-7] of these aspects of plasticity in bcc metals are available in the literature.

It is now widely accepted that the high Peierls stress for the motion of $(a/2)\langle 111 \rangle$ screw dislocations due to their non-planar core structure is responsible for the low-temperature plastic behaviour of bcc metals. Atomistic calculations of the screw dislocation core structure in bcc metals based on interatomic potentials do confirm the non-planar splitting of the core. Computer simulation studies of the screw dislocation motion are being attempted by several workers with a view to explain the experimental observations [3, 8]. In this regard, bcc alkali metals are of special interest due to their reliable interatomic potentials obtained from first principles. The present experimental study concerns the orientation and temperature dependence

of yield stress of potassium and its dilute alloys in the temperature range of 1.5 to 30 K. The orientation dependence of the low-temperature yield stress of potassium was reported earlier [9]. The purpose of this communication is to consider (a) further details relating to the applicability of the Schmid law of CRSS in the thermal and athermal regions of yield stress, and (b) alloying effects in the low-temperature deformation of potassium.

2. Experimental procedure

Potassium of 99.99% purity supplied by the Mines Safety Appliance Research Corporation, USA, was filled into oil-coated glass tubes using a procedure similar to that of Andrade and Tsien [10]. Single crystals were grown by the Bridgeman method and their orientations were determined by the Laue transmission method. The residual resistance ratio ($RRR = R_{293K}/R_{4.2K}$) of crystals thus prepared was ~ 200 . K-Na (0.1 and 0.25 at % Na) and K-Rb (1 at % Rb) alloys were prepared by mixing potassium with sodium and rubidium (both of 99.99% purity) in appropriate proportions under an argon atmosphere. Single crystals of the alloys were also grown as above and their residual resistance ratio was measured. The RRR values of K-0.1% Na, K-0.25% Na and K-1% Rb alloys were ~ 55 , 20 and 50, respectively.

Tensile specimens with a reduced gauge section (4 mm diameter and 30 mm length) were prepared by chemical polishing of the single crystal rods in a bath of 80% acetone and 20% methanol at 273 K. The specimens were then washed in petroleum ether and transferred to liquid nitrogen for storage before testing. Each specimen was mounted in the tensile grips using a special jig while the sample and grips were immersed in liquid nitrogen. The specimen was then quickly transferred to the tensile machine and the specimen chamber was evacuated immediately thereafter. Tensile tests were performed on a hard tensile

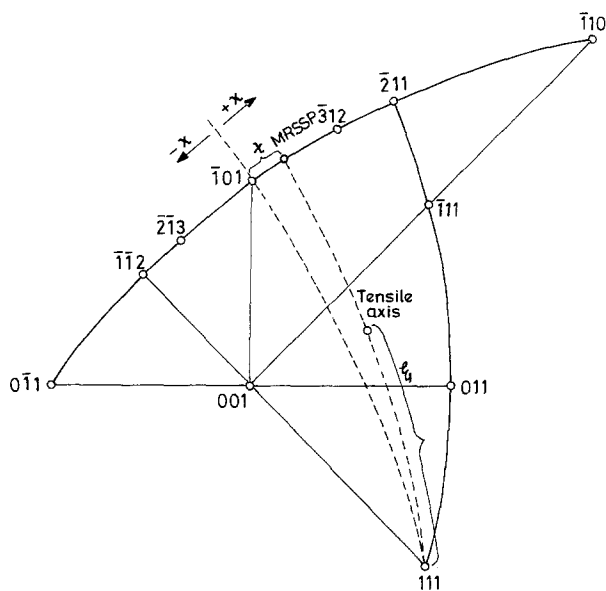


Figure 1 Part of [001] stereographic projection showing standard reference triangle and planes of [111] zone.

machine equipped with a ^4He cryostat. The test procedure consisted of recording the load against elongation curve up to about 0.1% plastic strain at each test temperature in the range of 1.5 to 30 K in the order of increasing test temperatures. The strain rate was $3.4 \times 10^{-4} \text{sec}^{-1}$ in all cases. The strain rate sensitivity of yield stress at each test temperature was measured through an increase in the strain rate by a factor of ten. The criterion employed in identifying the yield stress was the stress corresponding to an offset of 0.1% strain.

3. Results and discussion

As in previous studies on potassium [11–15], the yield stress is strongly temperature-dependent below $\sim 20 \text{K}$. To assess the validity of the Schmid law for slip, the question arises as to which slip system is to be considered. Identification of the operative slip systems in potassium by surface slip-line trace analysis has not yet been done except for the ambient temperature

deformation [10]. Hence several probable slip planes belonging to the zone of primary slip direction are considered for this purpose. A part of the standard [001] stereographic projection with the planes belonging to [111] zone is shown in Fig. 1. The critical resolved shear stress for slip on $(\bar{1}01)$ [111] (primary slip system) is referred to as the *first critical shear stress*, while that on the second most highly stressed $\{110\}$ [111] is the *second critical shear stress*. The maximum resolved shear stress plane is shown by the point of intersection of the great circle passing through the tensile axis and [111] with the [111] zone (Fig. 1).

3.1. $T < 20 \text{K}$ (temperature-dependent yield stress region)

3.1.1. Potassium

As already reported [9], the Schmid law of CRSS is not valid for potassium and the observed orientation dependence of the 0 K extrapolated MRSS values is in agreement with the theoretical calculations of Basinski and Duesbery [8]. In the interest of more direct comparison with the work on bcc transition metals, alternative representations of the results of this study on potassium are considered here. Fig. 2 shows the CRSS values of the primary $\{110\} \langle 111 \rangle$ slip system for the central region and corner orientations of the standard stereographic triangle at various temperatures. The orientation dependence of the 0 K extrapolated CRSS values are presented as CRSS against χ (see Fig. 1 for its definition) plots in Figs. 3 to 6. The thermal component of CRSS ($\tau_{0\text{K}} - \tau_{30\text{K}}$) has also been included in these plots. The data presented do not indicate a smooth variation of CRSS with χ . This could be due to some scatter in the experimental data and a complex orientation dependence of CRSS that may not be adequately represented through the consideration of χ only. Since the spread in the measured yield stresses of specimens with identical orientations is less than 10%, the latter is considered to be the major factor. From the data of Figs. 3 and 4 it is seen that the central region around $\chi = 0$

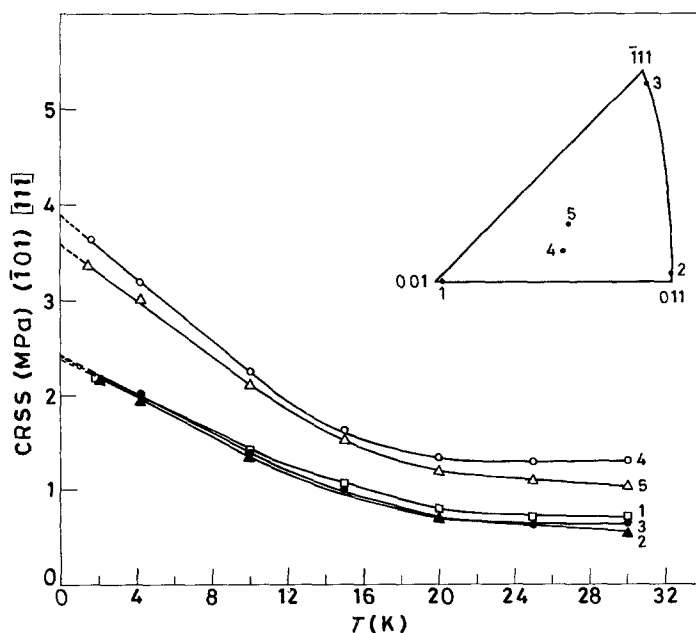


Figure 2 Temperature dependence of critical resolved shear stress for crystals of different orientations: (□) Crystal 1, (▲) Crystal 2, (●) Crystal 3, (○) Crystal 4, (△) Crystal 5.

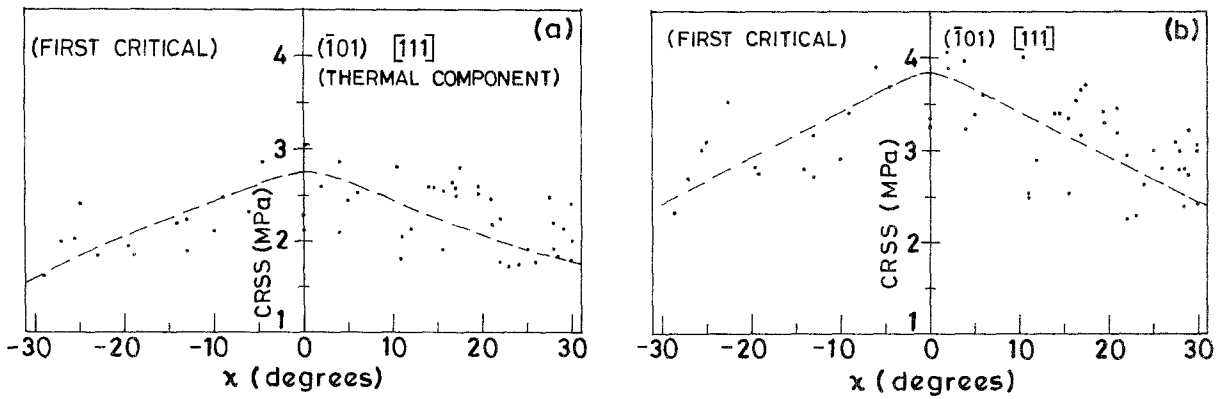


Figure 3 χ dependence of the 0 K extrapolated first critical shear stress: (a) thermal component, (b) applied stress.

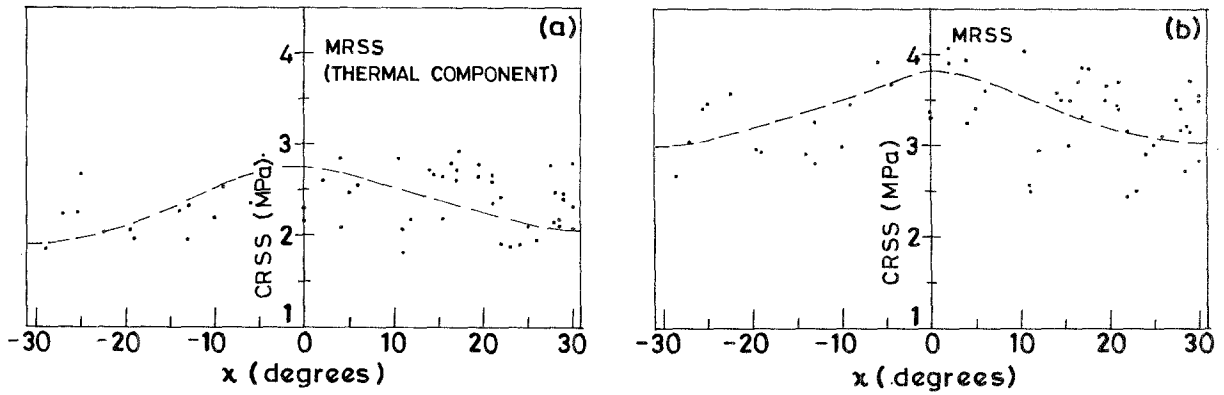


Figure 4 χ dependence of the 0 K extrapolated maximum resolved shear stress: (a) thermal component, (b) applied stress.

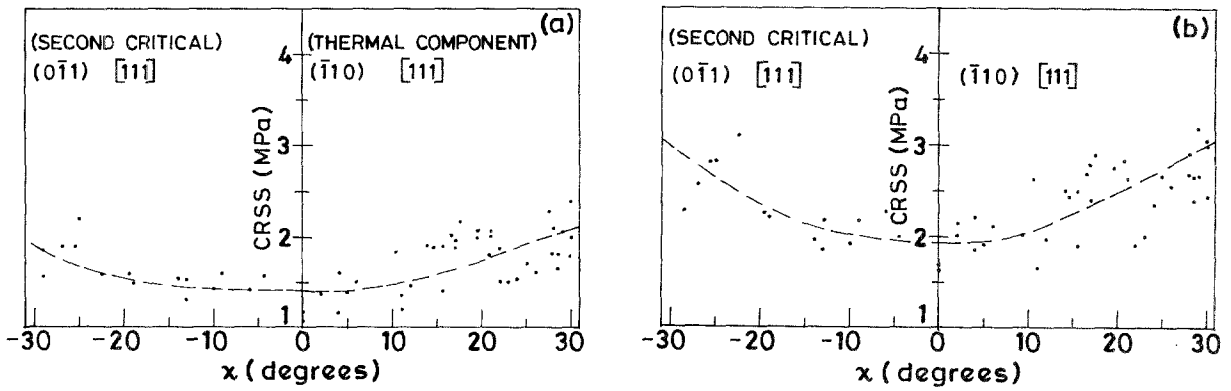


Figure 5 χ dependence of the 0 K extrapolated second critical shear stress: (a) thermal component, (b) applied stress.

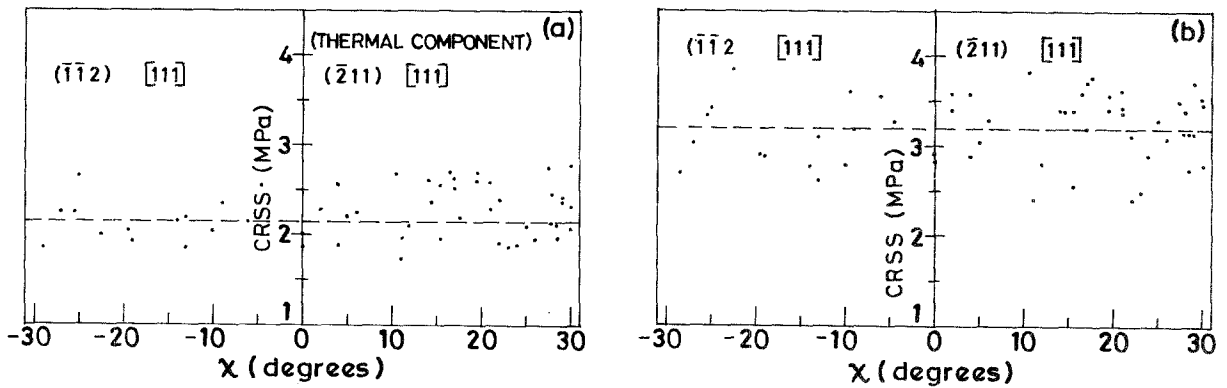


Figure 6 χ dependence of the 0 K extrapolated critical resolved shear stress for slip on $\{112\} [111]$: (a) thermal component, (b) applied stress.

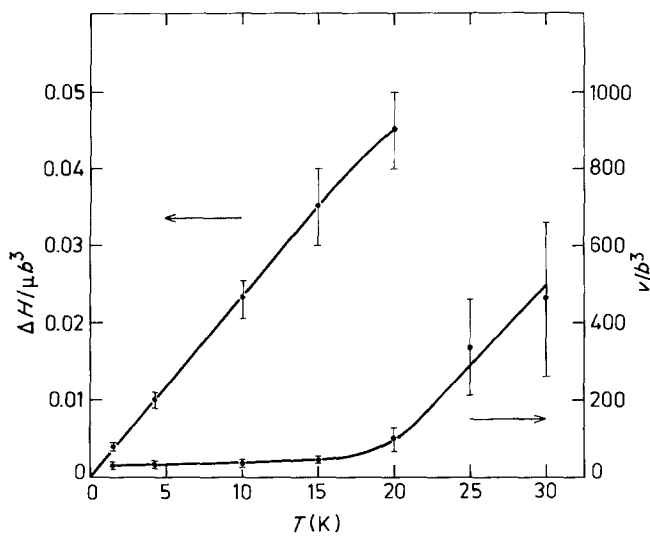


Figure 7 Temperature dependence of activation energy, ΔH , and activation volume, v , for plastic flow. Error bars represent standard deviations. μ is the $\langle 111 \rangle$ shear modulus and b the atom size.

corresponds to higher values of CRSS than the other regions. The opposite trend of lower CRSS values around $\chi = 0$ is evident from the second critical shear stress data given in Fig. 5. On the other hand, no systematic variation of CRSS with χ is evident from the data of Fig. 6 for the slip system $\{112\} \langle 111 \rangle$.

Assuming a simple rate equation for thermally activated flow through dislocation motion, the activation volume (v) and activation energy (ΔH) for low-temperature plastic flow were calculated. The data for activation parameters shown in Fig. 7 indicate that the activation volume is small ($\sim 30b^3$ where b is the atom size) and the activation energy increases linearly with temperature in the region where the yield stress is strongly temperature-dependent. These observations are in agreement with the Peierls mechanism wherein the rate-controlling factor is the formation of double kinks on screw dislocations. At temperatures above ~ 20 K, the thermal energy is sufficiently high to nucleate double kinks and the yield stress becomes athermal.

3.1.2. Alloying effects

Substitutional solutes (sodium and rubidium) were added to potassium to assess the solute effects on

low-temperature yield strength. From the data shown in Fig. 8, it is seen that the alloying leads to (i) a softening effect for flow, (ii) a lowering in the rate of change of CRSS with temperature, and (iii) a decrease in transition temperature for the onset of the athermal region of yield stress. In bringing about these changes, sodium is more effective than rubidium. It may be noted that the atom size difference between the solute and potassium is larger for sodium than for rubidium. The extent of softening near 0 K increases with increasing solute content within the investigated composition range. In the case of K-0.25% Na alloy, a mildly temperature-dependent CRSS region begins above 10 K and the CRSS becomes athermal only above ~ 50 K. Alloy softening has also been reported by Hands and Rosenberg [14] in polycrystalline potassium alloys, but only up to a sodium content of 0.01 at%. In contrast to the present observations, alloying additions in superpure transition metals lead to softening at intermediate temperatures and hardening in the very low temperature range, as well as in the athermal region [16, 17]. Further studies on the orientation and concentration dependence of alloying effects in potassium are clearly needed.

The alloy softening in potassium due to the alkali

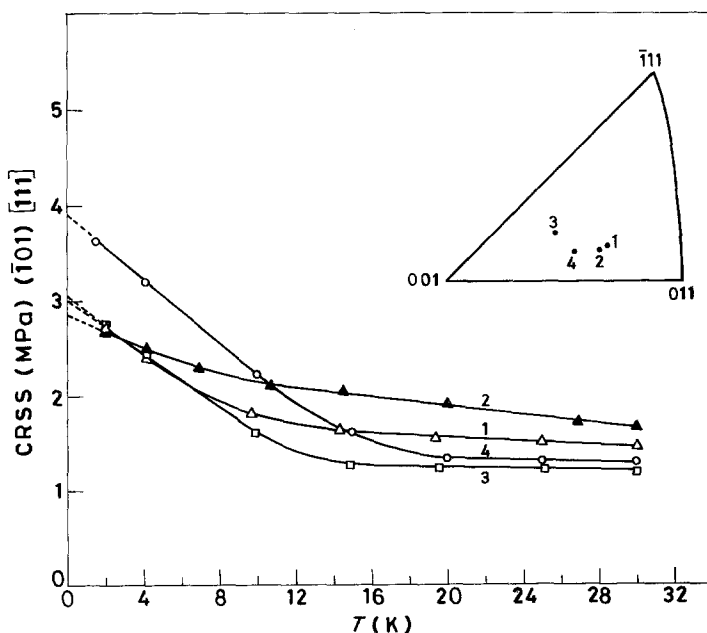


Figure 8 Temperature dependence of critical resolved shear stress for potassium and its alloys: (Δ) Crystal 1, K-0.1% Na; (\blacktriangle) Crystal 2, K-0.25% Na; (\square) Crystal 3, K-1% Rb; (\circ) Crystal 4, pure potassium.

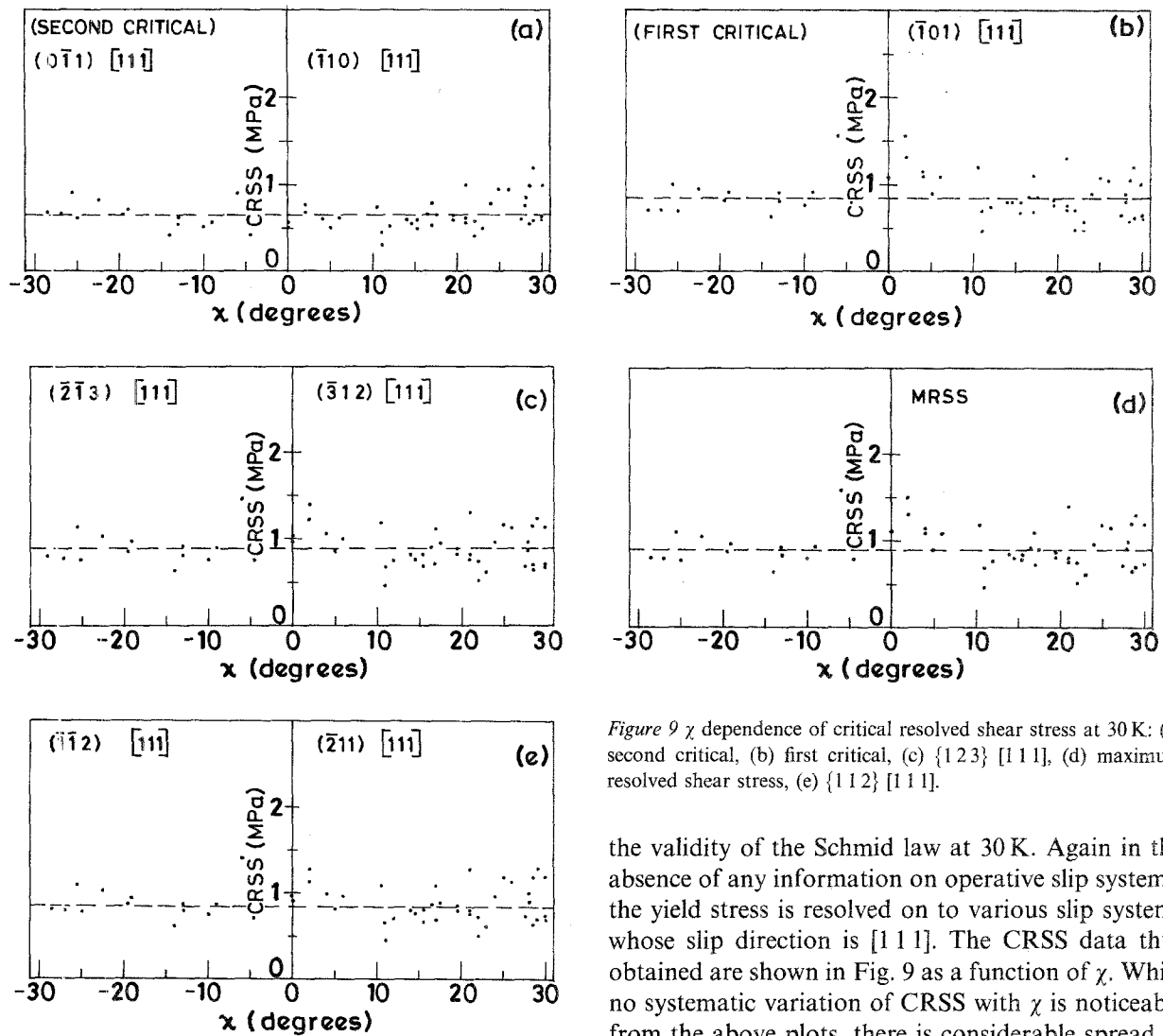


Figure 9 χ dependence of critical resolved shear stress at 30 K: (a) second critical, (b) first critical, (c) $\{123\}$ $[111]$, (d) maximum resolved shear stress, (e) $\{112\}$ $[111]$.

solute atoms is not likely to be an extrinsic effect such as scavenging of interstitial impurities from the solid solution by the substitutional solute. In view of the established importance of the Peierls mechanism in the low-temperature deformation of bcc metals, it is reasonable to consider alloy softening as an intrinsic phenomenon. As a result of interaction between solute atoms and a screw dislocation, the nucleation of double kinks in an alloy can be easier than in a pure metal [18, 19] and alloy softening will then be expected.

3.2. $T = 30$ K (athermal yield stress region)

In the temperature range where the yield stress becomes temperature-independent, the mobilities of screw and edge dislocations are similar and all the special characteristics of low-temperature plasticity are likely to disappear. For example, the orientation dependence of the CRSS and yield asymmetry vanish in several bcc transition metals [20], implying that the Schmid law of CRSS is valid in the athermal region. The present observations in potassium do not seem to be in full agreement with those of bcc transition metals. The data of Fig. 2 indicate that the CRSS values for orientations in the central region of the stereographic triangle are higher than those of the corner orientations, even in the athermal region of yield stress. Hence an attempt has been made to assess

the validity of the Schmid law at 30 K. Again in the absence of any information on operative slip systems, the yield stress is resolved on to various slip systems whose slip direction is $[111]$. The CRSS data thus obtained are shown in Fig. 9 as a function of χ . While no systematic variation of CRSS with χ is noticeable from the above plots, there is considerable spread in the CRSS data. Assuming that the variations in CRSS values are only due to scatter, the arithmetic mean ($\bar{\tau}$), standard deviation (s) and coefficient of variation ($s/\bar{\tau}$) have been calculated and compared with those for 0 K in Table I. What is disturbing from this comparison is that the coefficient of variation in the CRSS data at 30 K is larger than that at 0 K by at least a factor of two. This suggests that there may be some orientation dependence of CRSS even at 30 K, and Schmid law may not be valid just as in the lower-temperature range. If this were true, it would be difficult to rationalize this effect in view of the planar core of the edge dislocation and the similar mobilities of edge and screw dislocations in the athermal region. Even if an alternate mechanism of solute atom-dislocation interactions is considered to account for the yield stress in the athermal region, the reason for the above trend in the CRSS data remains uncertain.

4. Conclusions

1. The Schmid law of CRSS for slip in potassium is not valid for the temperature-dependent region of yield stress. The observations in the temperature-dependent region of yield stress are in agreement with the Peierls stress for screw dislocation motion.

2. In the athermal region of yield stress, the CRSS values vary widely with orientation. While no systematic variation of CRSS with the angle χ is evident, the extent of change in CRSS with orientation is larger

TABLE I Statistical analysis of CRSS data of potassium, assuming the variations to be due to scatter only

Slip system	$T = 0\text{ K}$			$T = 30\text{ K}$		
	Arithmetic mean CRSS, $\bar{\tau}$ (MPa)	Standard deviation, s	Coefficient of variation, $s/\bar{\tau}$ (%)	Arithmetic mean CRSS, $\bar{\tau}$ (MPa)	Standard deviation, s	Coefficient of variation, $s/\bar{\tau}$ (%)
($\bar{1}01$) [111] (first critical)	3.12	0.4602	14.8	0.85	0.2509	29.5
{ 110 } [111] (second critical)	2.34	0.4008	17.1	0.67	0.2113	31.5
MRSS	3.32	0.4196	12.6	0.90	0.2254	25.0
{ 112 } [111]	3.18	0.3888	12.2	0.84	0.3556	42.3
{ 123 } [111]	3.23	0.4082	12.6	0.89	0.3127	35.1

than that of the temperature-dependent region. Thus the validity of the Schmid law may be questionable even in the athermal region where the mobilities of edge and screw dislocations are similar.

3. Solid solution softening is observed in potassium single crystals in the temperature-dependent region of yield stress on adding substitutional solutes of sodium and rubidium. The larger the atom size difference between the solute and potassium, the greater is the softening effect near 0 K.

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