Temperature dependence of the electrical conductivity of amorphous V_xSi_{1-x}

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We present results for the temperature dependence of electrical conductivity for amorphous V_xSi_{1-x} alloys. The alloys investigated span the composition range from $x=0.5$ to 0.1. For the alloys with more than 20 at. % V, the temperature dependence could be successfully fitted with use of the theories of quantum interference effects, and values for the spin-orbit and inelastic scattering rates are extracted from the fits. As the concentration of V is decreased, there is evidence for a metal-insulator transition seen at around 15 to 13 at. % V. The temperature dependence of the conductivity is surprisingly similar for all the alloys on the metallic side of the transition, showing a clear $T^{1/2}$ dependence at the lowest temperatures while the insulating $V_{0.1}Si_{0.9}$ alloy shows evidence for variable-range-hopping conduction. The $V_{0.13}Si_{0.87}$ alloy, which is right at the transition, exhibits an unusual temperature dependence. The sample is metallic and seems to follow a $T^{1/3}$ dependence at low temperatures.

INTRODUCTION

A number of transition-metal–metalloid amorphous alloys have been studied because they exhibit a metal-insulator transtion at around 80–90 at. % metalloid. Here we present results of a study on the V-Si system. It is a system which has not been studied in detail in the past and we have used it to investigate quantum-interference effects across a wide range of conductivities through the metal-insulator transition. There have been many reports of quantum-interference effects in amorphous metal alloys with conductivities around 5000 $\Omega^{-1}\,m^{-1}$, the Cu-Ti system, for example.[1] But there have not been many studies on systems which have lower conductivities where we may expect the theories of quantum interference or "weak" localization—which are only strictly valid in the weak-scattering limit—to break down. These alloys may be said to be in a "strong"-localization regime

Much of the work that has been done on lower-conductivity systems has concentrated on the region very close to the metal-insulator transition and on the low-temperature $\sqrt{T}$ dependence of the conductivity.[2,3] This $\sqrt{T}$ dependence is due to electron-electron correlations in the presence of the interference effects. Although it is often considered as a separate contribution to the conductivity from the quantum-interference effects, it is in fact a quantum-interference effect itself.[4] Castellani *et al.*[5] argue that for an "interaction"-driven metal-insulator transition the $\sqrt{T}$ dependence will persist right through the transition.

Here we see how the quantum-interference effects can be applied to alloys which have conductivities ranging from well above to well below the Ioffe-Regel limit, $E_F\tau_{tr}\sim 1$. However, close to the transition we see a marked deviation from the usual $\sqrt{T}$ dependence, and there is some evidence that a $T^{1/3}$ dependence is seen. We have also tried to fit our data to a theory of "$2k_F$" scattering, which includes both the "weak"- and "strong"-localization regimes and also predicts an Anderson-type transition at a critical value of $E_F\tau$.[6] (Here we make distinction between τ_{tr}, a transport lifetime determined from the resistivity, and τ, the one-electron relaxation time.)

Some work on V-Si has already been done by Ousset *et al.*[7] Their work was on thin films which were believed to be two-dimensional (2D) as far as the interference effects were concerned (thickness ≤ 500 Å), and so a direct comparison with our results is not possible, except that we would expect the inelastic and spin-orbit scattering rates extracted from the theoretical fits to the data to be similar. They see some phase separation for samples with less than 20at. % V and suggest this is why they do not see a metal-insulator transition around the expected 15 at. % V concentration. However, they do note a large increase in the magnetoresistance as the Si concentration approaches 85%, and they argue that this is evidence for the appearance of "strong"-localization effects. We do not see any evidence for phase separation in transmission electron microscopy (TEM) studies, and we do see a metal-insulator transition around 13 at. % V. However, we have three-dimensional samples (thickness ~ 3000 Å); it is possible that Ousset *et al.* do not see a metal-insulator transition because their samples are 2D in character.

EXPERIMENTAL DETAIL

The alloys were sputtered onto a room-temperature silica substrate from an alloy target made from 99.9999% pure Si and 99.999% pure V. The thicknesses of the films were in the range 0.2–0.8 μm, and the compositions were determined using energy-disperse x-ray analysis (EDAX). Measurements of the electrical conductivity were made over the temperature range 1–80 K by a four-probe dc method.

RESULTS AND DISCUSSION

In Figs. 1(a) and 1(b) the resistance of V_xSi_{1-x} normalized to the value at 80 K is shown versus temperature. There is a clear difference in behavior between alloys with $x<0.15$ and those with $x\geq 0.15$. The alloys with $x>0.15$ are metallic with a finite resistivity extrapolated to absolute zero, while the resistivity of the $x=0.10$ alloy diverges at low temperatures and the alloy is clearly insulating. The temperature dependence for the $x=0.13$ alloy is much stronger than that of the other metallic alloys, but from Fig. 1(b) we see that it appears to extrapolate to a nonzero conductivity at absolute zero and is therefore metallic. This suggests that for $x\geq 0.15$ the alloys are in the "weak"-localization regime, for $x<0.13$ the alloys are insulators, while for x around 0.13 the alloys are in the "strong"-localization regime. The metal-insulator transition is clearly in the vicinity of $x\sim 0.13$. In the following we will first consider the insulating, then the "weak"-localization, and finally the "strong"-localization regimes.

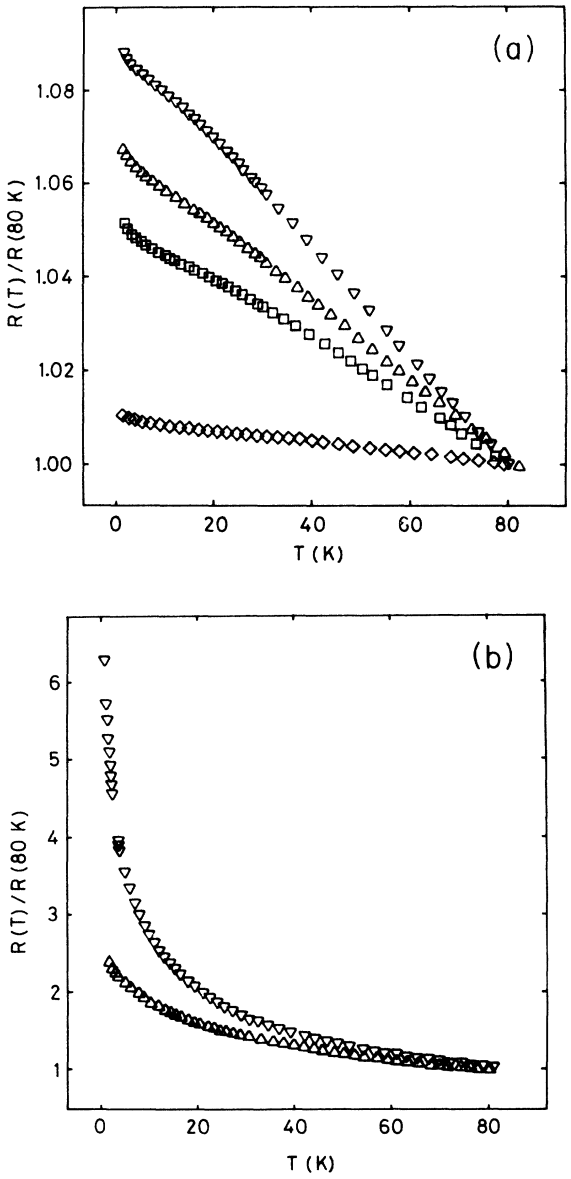

FIG. 1. (a) The resistance of V_xSi_{1-x} normalized to the resistance at 80 K vs temperature. $x=0.50$ (◇), 0.25 (□), 0.20 (△), and 0.15 (▽). (b) The resistance of V_xSi_{1-x} normalized to the resistance at 80 K vs temperature. $x=0.13$ (△) and 0.10 (▽).

In Fig. 2 we have plotted the logarithm of the resistance for the $x=0.1$ alloy normalized to its value at 80 K against $T^{-1/4}$. A linear dependence is seen for temperatures below about 20 K, which is a strong indication of the presence of variable-range hopping, where

$$\sigma = Ae^{-[T_0/T]^{1/4}}, \tag{1}$$

as we would expect on the insulating side of the transition at low temperatures.[8]

In Fig. 3 we show the conductivity for the alloys $x=0.5$, 0.25, 0.15, and 0.10. We have fitted the data to the theories of "weak" localization and electron-electron interaction effects. This sort of analysis has been successfully applied to a number of amorphous metal alloys in the past.[1,9,10] The form of the temperature dependence of the conductivity due to quantum-interference effects is[9]

$$\Delta\sigma = \frac{e^2}{2\pi^2\hbar D^{1/2}}\left[3\left[\frac{1}{\tau_{s.o.}}+\frac{1}{4\tau_i}\right]^{1/2}-\left[\frac{1}{4\tau_i}\right]^{1/2}\right], \tag{2}$$

where $\tau_{s.o.}$, τ_i, and D are the spin-orbit and inelastic relaxation times and the diffusion constant, respectively. Only τ_i is temperature dependent, and it assumed for this analysis that it is dominated by electron-phonon scattering, the temperature dependence of which is $\tau_i=\beta T^{-2}$.[9] The contribution to the conductivity in the weak-localization regime due to interaction effects is[9]

$$\Delta\sigma = \frac{1.3e^2}{4\pi^2\hbar}\left[\frac{4}{3}-3F^*-\frac{2}{\ln(T_0/T)}\right]\left[\frac{k_BT}{2\hbar D}\right]^{1/2}. \tag{3}$$

Here T_0 is a characteristic temperature of the order of the Fermi temperature. $F^*=F-\lambda$, where F and λ are

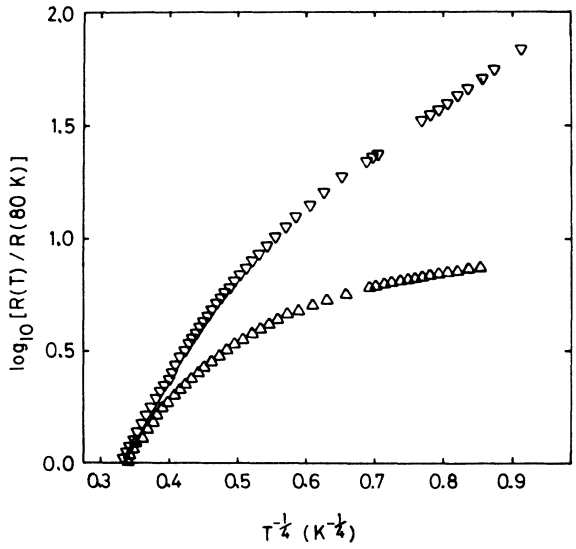

FIG. 2. The logarithm of the resistance normalized at 80 K vs $T^{-1/4}$ showing a linear region at low temperatures for $x=0.10$. $x=0.10$ (▽) and 0.13 (△).

the electron-electron and electron-phonon coupling constants, respectively. F^* should vary little and be close to zero in the weak-localization regime, and so in this analysis we have set it equal to 0.[9]

Equations (2) and (3) can be combined to take the form

$$\Delta\sigma=\frac{e^2}{2\pi^2\hbar}[3(A+BT^2)^{1/2}-(BT^2)^{1/2}+CT^{1/2}], \quad (4)$$

$$\text{where } A=\frac{1}{\sqrt{D\tau_{s.o.}}},$$

$$B=\frac{1}{\sqrt{4D\beta}},$$

and

$$C=0.65\left[\frac{4}{3}-3F^*-\frac{2}{\ln(T_0/T)}\right]\left[\frac{k_B}{2\hbar D}\right]^{1/2}.$$

This expression is fitted to the data for all samples, and from the values of A, B, and C we can extract values for $\tau_i=\beta T^{-2}$, $\tau_{s.o.}$ and D, having assumed F^* to be zero. In Fig. 3 the chained and solid lines are the contributions to the theoretical fit from localization and interaction effects, respectively. For clarity, the combined fit is not shown; however, within the size of the points, the fit follows the data. The values of the scattering times and the diffusion constants are shown in Table I. Also shown in Table I are the values of D, τ_i, and $\tau_{s.o.}$ obtained by Ousset *et al.*[7] from their magnetoresistance studies on V_xSi_{1-x}. We can see that the values are very similar to

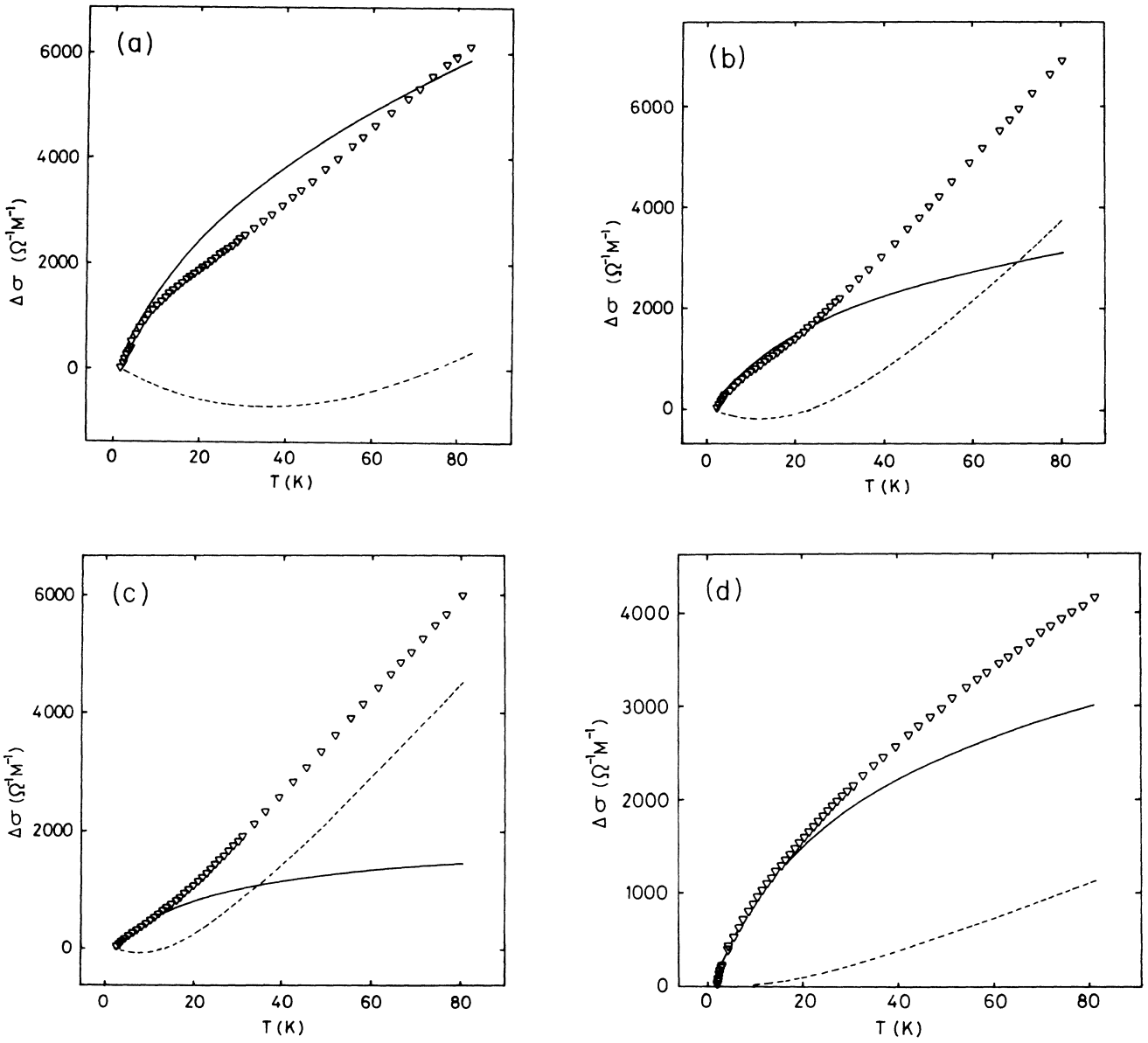

FIG. 3. The change in conductivity for $x=0.5$ (a), 0.25 (b), 0.15 (c), and 0.10 (d) at low temperatures. The chain line is the localization contribution to the fit, and the solid line is the $\sqrt{T}$ interaction contribution.

TABLE I. Values of spin-orbit scattering relative rate τ_{so}^{-1} and inelastic scattering relaxation rate ($\tau_i = \beta T^{-2}$). Values are also given for diffusion coefficient D and resistivity ρ at 4.2 K for the range of composition of V_xSi_{1-x} that has been investigated. An asterisk indicates our data. A dagger indicates data taken from Ref. 7.

Composition	β (sk^2)	τ_{so}^{-1}(s^{-1})	D (m^{2}s^{-1})	ρ ($\mu\Omega$ cm)
*$V_{50}Si_{50}$	2.4×10^{-9}	1.1×10^{12}	0.8×10^{-5}	170
*$V_{25}Si_{75}$	1.2×10^{-9}	2.57×10^{11}	1.4×10^{-5}	720
*$V_{15}Si_{85}$	5.2×10^{-8}	1.85×10^{11}	3.8×10^{-5}	1,440
*$V_{10}Si_{90}$	2.3×10^{-8}	3.85×10^{9}	1.6×10^{-5}	1.23×10^{5}
†$V_{48}Si_{52}$	$\sim2\times10^{-9}$	1.4×10^{12}	8×10^{-5}	345
†$V_{40}Si_{60}$	$\sim2\times10^{-9}$	1.0×10^{12}	6×10^{-5}	433
†$V_{25}Si_{75}$	$\sim1\times10^{-9}$	6.7×10^{11}	4×10^{-5}	646

our results. The inelastic-scattering times are fairly constant across the composition range, and similar to values obtained in many studies on many different systems.[11] The spin-orbit scattering times are typical for an alloy containing a relatively "heavy" element, V, and increase as the concentration of the V is decreased, as we might expect, since the strength of the spin-orbit interaction is related to the atomic number of the scatterer.

The $\sqrt{T}$ interaction contribution to the fits progressively decrease as the critical concentration for the metal-insulator transition is approached. In these fits, this arises simply from a corresponding increase in the magnitude of the diffusion constant.

For the $x=0.10$ alloy, also shown in Fig. 3, there is a sudden increase in the magnitude of the $\sqrt{T}$ interaction contribution and a corresponding drop in the localization contribution. This sample is on the insulating side of the transition and so we would expect the quantum-interference fits to break down. We can, of course, obtain a reasonable three-parameter fit, but the parameters are not physical. In Table I we have still included the values of the inelastic- and spin-orbit scattering times along with the diffusion constant, but only to show that there is a distinct discontinuity in the composition dependence of these parameters.

The $V_{0.13}Si_{0.87}$ alloy, which is close to the transition, also cannot be fitted by the weak-localization theories. We have considered a number of theories which might fit the temperature dependence. First, Finkelstein[12] has argued that $T^{1/3}$ dependence might be observed close to the metal-insulator transition, although Castellani *et al*[5] discuss a $\sqrt{T}$ dependence of the form

$$\Delta\sigma=\sigma_0+m^{1/2}$$

in the weak-scattering limit, but changing to

$$\sigma\propto T^{1/2}$$

close to the transition. Their arguments involve considering the interaction contribution to the conductivity to all orders in the electron-electron coupling strength, but quantum-interference effects to only first order in $(1/E_F\tau)^2$. The data for $V_{0.13}Si_{0.87}$ does not show a $\sqrt{T}$ dependence at low temperatures. However, we have plotted the data against $T^{1/3}$ in Fig. 4 and this shows evidence for a $T^{1/3}$ dependence of the conductivity up to quite high temperatures.

Morgan *et al.*[6] have taken the other extreme and neglected the interaction effects, but considered how so-called "$2k_F$ scattering" can lead not only to "weak"-localization effects but also to an Anderson transition at a critical value of $E_F\tau$. This theory has been applied to a number of different systems which show "strong"-localization effects or an Anderson transition. For example, it was shown to give the same quality of fit as the weak-localization fits for the amorphous alloy Ca_xAl_{1-x}.[13] This alloy has a resistivity which peaks at 450 $\mu\Omega$ cm for $x=0.4$ and has very weak spin-orbit scattering. The expression Morgan *et al.* obtain for the resistivity has the form[14]

$$\rho=\rho_B\left[\frac{1+\frac{\tau_B}{2\tau}\frac{y^3}{x}F_{\rm MHP}^{1/2}(y)}{1-\frac{3}{64}xy^3F^{1/2}(y)F_{\rm MHP}^{1/2}(y)}\right].$$

Here τ is the total one-electron energy relaxation time $y=\hbar/\tau_T E_F$ $\tau_T^{-1}=\tau^{-1}+\tau_i^{-1}$, and $x=\hbar/\tau E_F$; ρ_B is the uncorrected Boltzmann resistivity. The functions F and $F_{\rm MHP}$ are given by

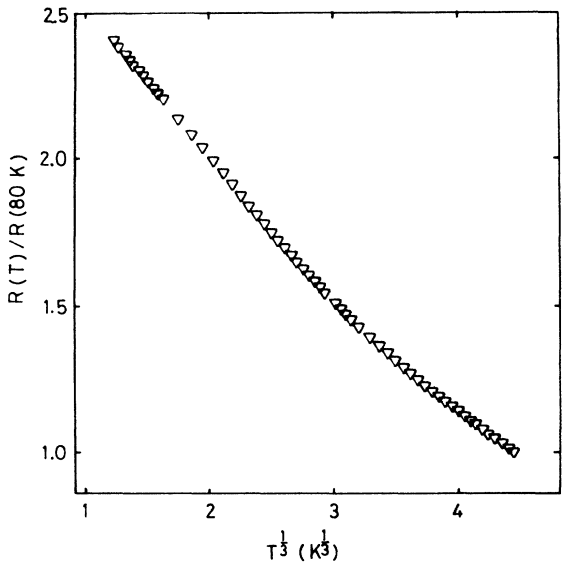

FIG. 4. Resistivity vs the cube root of the temperature for $V_{13}Si_{87}$.

$$F^{1/2}(y)=\ln\left[\frac{(1+y^2)^{1/2}+1+\sqrt{2}[(1+y^2)^{1/2}+1]^{1/2}}{(1+y^2)^{1/2}+1-\sqrt{2}[(1+y^2)^{1/2}+1]^{1/2}}\right],$$

$$F^{1/2}_{\mathrm{MHP}}(y)=\ln\left[\frac{(1+y^2)^{1/2}+1+\sqrt{2}(1+y^2)^{1/2}+2y(A/1-A)^{1/2}[(1+y^2)^{1/2}-1]^{1/2}+2y^2(A/1-A)}{(1+y^2)^{1/2}+1-\sqrt{2}(1+y^2)^{1/2}+2y(A/1-A)^{1/2}[(1+y^2)^{1/2}-1]^{1/2}+2y^2(A/1-A)}\right]^2.$$

here $A=\left[1-\frac{\tau_T}{\tau}\right]$.

We have attempted to fit our data for the $x=0.13$ alloy, which is in the strong-localization regime, using this theory and including the $\sqrt{T}$ contribution from the interaction effects. However, it is impossible to fit this model to the data for $V_{13}Si_{97}$. The theory itself does not include the effects of spin-orbit scattering, and since this cannot be neglected in this alloy system it is, therefore, an unfair test of the theory.

CONCLUSION

We have observed a metal-insulator transition in V_xSi_{1-x} at $x\sim0.13$. For samples with $x<0.13$ we have been able to fit the normal weak-scattering quantum-interference theory and extract values for τ_i and $\tau_{s.o.}$. The $V_{13}Si_{97}$ alloy is close to the metal-insulator transition. We have been unable to fit the theories of quantum interference to this alloy. The alloy shows evidence of $\Delta\rho\propto T^{1/3}$, and we believe this alloy to be in the "strong" localization regime. The $V_{10}Si_{90}$ is clearly insulating, and shows evidence of variable-range hopping.

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