

Electrical resistivity of liquid nickel-lanthanum and nickel-cerium alloys

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The high-temperature melting points of transition metals and the extreme reactivity of rare-earth metals at high temperature explain why very few results exist on the physical properties of this kind of alloy. Except for some papers of Solodovnikov *et al.*, no paper on the electronic properties of transition-metal-rare-earth alloys have been published to our knowledge. The scarce pure-metal results are often contradictory. The electrical resistivity of nine liquid lanthanum-nickel alloys (up to 60 at. % nickel) and of six cerium-nickel alloys (up to 53 at. % nickel) has been measured. The raw experimental results had been presented earlier. The concentration dependence of the resistivity is discussed in the framework of the extended Faber-Ziman theory of Dreirach *et al.* in terms of structure factors and form factors. Following a hard-sphere description, we used the Ashcroft-Langreth formula to compute the partial structure factors. The form factors have been deduced by taking transition- and rare-earth-metal model potentials of the Heine-Abarenkov-Animalu type which incorporate formally the *s-d* and the *s-f* hybridization in the energy band of the lanthanides. Alternatively, we also compute a *t*-matrix form factor expressed in terms of phase shifts. The model-potential and *t*-matrix-form-factor calculations are compared to the experimental resistivity.

I. INTRODUCTION

It is largely agreed that the electrical transport in simple metals has been resolved from a theoretical point of view. In liquid alloys the transport properties are well described by the nearly-free-electron theory with the Faber-Ziman formula.¹ However, for transition and rare-earth metals, the pseudopotential theory developed before 1969²⁻⁴ fails. Harrison⁵ introduced a generalized pseudopotential method for *d*-band metals taking into account a hybridization of the *d* band with the free-electron-like conduction band. Animalu⁶ introduced the transition-metal model potential (TMMP) by extending the concept of "quantum defect" to determine the parameters of a Heine-Abarenkov-type model potential. He showed that the *l*=2 model-potential parameter A_2 reflects the Ziman-Heine-Hubbard model of *s-d* hybridization. Upadhyaya and Animalu⁷ proposed a rare-earth-metal model potential (REMMP) which incorporates formally the *s-f* hybridization of the energy band of the lanthanides through an *l*=3 model-potential-well depth of the resonance form: $A_3(E) = \frac{1}{2}W_f/(E_f - E)$, where W_f and E_f are, respectively, the width and the position of the narrow *f* band. An alternative solution is to use the "extended Faber-Ziman formula."⁸ The pseudopotential form factor is simply replaced by a *t*-matrix form factor expressed in terms of phase shifts which are computed by using a suitable muffin-tin potential. The key quantity is the number N_c of conduction electrons by ion. A first guess would be that N_c equals the valency as

has been proposed by Waseda,⁹ but Delley *et al.*^{10,11} analyzing band-structure calculations for solid lanthanum gave evidence that for trivalent rare-earth elements, N_c should be as low as 0.5. Delley *et al.*¹² explain at least qualitatively the temperature coefficient across the lanthanide series.

The structure for an alloy is described by three partial structure factors. In a first approximation they can be computed¹³ assuming the liquid is a mixture of randomly distributed hard spheres with different diameters. After recalling the basic formula in Sec. II we discuss our experimental method in Sec. III, and we present our measured resistivities as a function of temperature and composition in Sec. IV. We compare, in Sec. V, our results to the values calculated with hard-sphere structure factors using different sets of phase shifts and the REMMP.

II. THEORY

Ziman¹⁴ has shown that the electrical resistivity of a pure liquid metal can be computed using the expression

$$\rho = (3\pi\Omega_0/4e^2\hbar^3k_F^6) \int_0^{2k_F} a(q)[v(q)]^2 q^3 dq, \quad (1)$$

where $a(q)$ is the static structure factor, $v(q)$ the pseudopotential (or model potential) form factor, Ω_0 the atomic volume, and k_F the Fermi wave vector. Other symbols have their customary meaning. This formula can be extended to binary alloys by replacing the product $a(q)[v(q)]^2$ in the integral of (1) by

$$[v_1(q)]^2[c(1-c) + c^2a_{11}(q)] + [v_2(q)]^2[c(1-c) + (1-c)^2a_{22}(q)] + 2v_1(q)v_2(q)c(1-c)[a_{12}(q) - 1]. \quad (2)$$

Here c is the atomic fraction of constituent 1, $v_i(q)$ the form factor of species i in the alloy, and the $a_{ij}(q)$ are the Faber-Ziman partial structure factors. In this paper we used the TMMP proposed by Animalu⁶ for nickel and the REMMP of Upadhyaya and Animalu⁷ for lanthanum. We simply replace $v_i(q)$ in the Faber-Ziman¹ formula by the t -matrix form factor $t_i(q, E_F)$; we then obtain what is generally known as the extended Faber-Ziman formula.⁸ Our calculations have been performed using the phase shifts (which enter into the t matrix) given by Dreirach *et al.*,⁸ Waseda,⁹ and Delley and Beck.¹¹ The radius of the Fermi sphere k_F is related to the number of conduction electrons N_c instead of the valence Z by

$$k_F^3 = 3\pi^2 N_c / \Omega_0(T). \quad (3)$$

The Fermi energy E_F is expressed as a function of the bottom energy E_b :

$$E_F = E_b + \hbar^2 k_F^2 / 2m^*. \quad (4)$$

The one-particle t matrix $t(q, E_F)$ describing the amplitude for electron-ion scattering at energy E_F and momentum transfer q is expressed by the phase shifts $\eta_i(E_F)$:

$$t(q, E_F) = \frac{-2\pi\hbar^3}{m(2mE_F)^{1/2}} \frac{1}{\Omega_0} \left[\sum_l (2l+1) \sin[\eta_l(E_F)] \times \exp[i\eta_l(E_F)] \right] \times P_l(\cos\theta). \quad (5)$$

The phase shift values at E_F are taken from Delley and Beck, Fig. 1.¹¹ However their renormalized phase shifts have not been published. Our calculations have been performed with hard-sphere partial structure factors. At each temperature the hard-sphere diameters are deduced from the experimental densities of the pure metals compiled by Crawley¹⁵ and from their packing fraction given by the Waseda empirical law:

$$\eta_i(T) = A_i \exp(-B_i T), \quad (6)$$

where the parameters A_i and B_i have been taken from Waseda's book.⁹ The hard-sphere diameters are held constant with composition. They are given by

$$\sigma_i^3(T) = [8\eta_i(T)\Omega_i(T)/\pi]. \quad (7)$$

However, calculations were performed at 700°C and it is not sure that formula (6) can be used at this temperature since the parameters have been obtained in the liquid phase, i.e., above 1450°C for liquid nickel, and that for liquid lanthanum and cerium the temperature coefficient B is very important. The extrapolated pure-metal values of the packing fraction at 700°C are too high (about 0.54) and may be unphysical. We prefer to postulate that, for deep eutectic systems, the packing fraction remains constant on the liquidus curve. The corrected packing fractions we used are obtained from

$$\eta_i(T) = A_i \exp[-B_i(T - T_{\text{liq}} + T_{mi})], \quad (8)$$

where T_{liq} is the liquidus temperature at the given concentration and T_{mi} is the pure-metal melting point. In the alloy we have taken into account the modification of the mean atomic volume $\Omega_0(T)$ and of the Fermi wave vector k_F

$$k_F^3 = 3\pi^2 Z / \Omega_0(T). \quad (9)$$

Z and $\Omega_0(T)$ are, respectively, the mean valence and the mean atomic volume of the alloy obtained by a linear interpolation of the pure-metals values (for the rare earth we take N_c instead of Z).

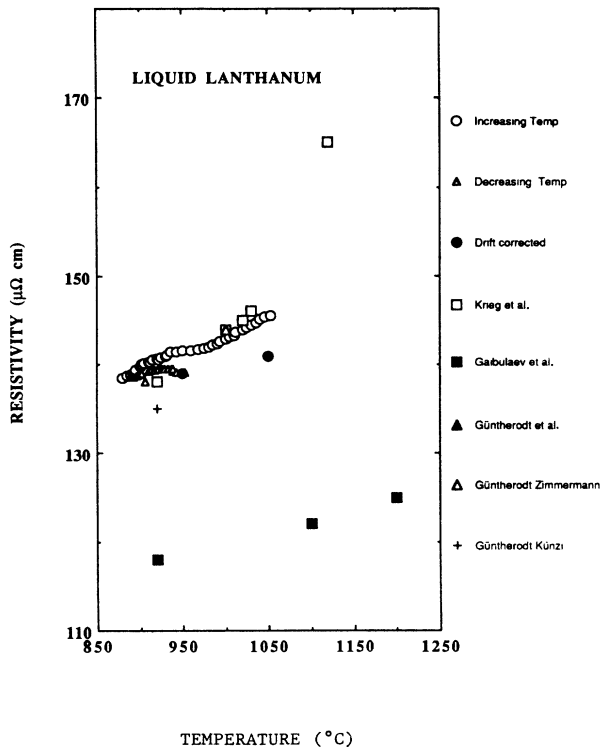


FIG. 1. Electrical resistivity of liquid lanthanum. The following have been represented: experimental values measured by decreasing temperature; experimental values measured by increasing temperature; drift corrected values; values of Gaibulaev (Ref. 21); Krieg *et al.* (Ref. 20); Güntherodt *et al.* (Ref. 25); Güntherodt and Zimmerman (Ref. 23); Güntherodt and Künzi (Ref. 22).

III. EXPERIMENTAL METHOD

Resistivity measurements were performed by the four-probe method using a quartz (fused silica) cell fitted with tungsten electrodes. The accuracy of the electrical measurement of the resistivity is estimated to be 0.5% and that of the temperature 0.4%. The geometrical constant of the cell was calibrated by measuring the resistivity of triple distilled mercury. Full experimental details have been described by Gasser.¹⁶ However the rare-earth metals are very corrosive and react with silica (and alumina) at high temperatures. (Other authors have measured the electrical resistivity of pure rare earth in conducting tan-

talum cells; however this technique cannot be used because of the chemical reaction of nickel with tantalum.)

In our case a chemical reaction with the cell has been made evident by preliminary experiments; indeed at constant temperature the measured resistance grows slowly with time. For lanthanum alloys we have first determined that this phenomena disappears below 800°C, so we only made measurements below this temperature. For cerium alloys the drift could not be completely eliminated, even at lower temperatures, but its effect on the resistivity was estimated to 1.4% by day and permitted the correction of our raw measurements. We observed after the end of the experimental runs the formation (on the internal face of the capillary) of a solid film of undetermined composition which reduces the diameter of the capillary, and hence, the geometrical constant of the cell. This is consistent with the drift observed if the film is less conducting than the liquid alloy. This phenomenon could be explained by a chemical reaction between cerium and silica; the film being probably a cerium oxide and silicium being introduced in the alloy. The ternary phase diagram of Ni-Ce-Si is not known, but the binary phase diagram Ce-Si and Ni-Si indicates that the small amount of silicium is probably not soluble in the liquid alloy at the measured temperature and probably "floats" on the alloy in the principal and auxilliary storage tank. We did not observe a measurable change of resistance when the 1 mm diameter capillary was cleared and filled again. This indicates that the observed drift is certainly more due to a geometrical effect than to a chemical effect.

We handled and weighted lanthanum and cerium in a glove box to prevent their reaction with air. The composition has been modified by adding weighted amounts of nickel. Because of its high melting point (nickel must be fully dissolved in liquid cerium and lanthanum) we mixed thoroughly the liquid alloy and cleared out the capillary by applying successively vacuum or argon over the sample.

IV. EXPERIMENTAL RESULTS

Except for the work of Solodovnikov *et al.*^{17,18} and our raw experimental results presented by Kefif and Gasser,¹⁹ there exists, to our knowledge, no other experimental measurement (in the liquid state) on the electrical resistivity of an alloy of a lanthanide rare-earth metal with a transition metal. For the pure rare earth metals, the experimental data are scarce and sometimes very different. We present below our measurements on the electrical resistivity of liquid lanthanum and liquid cerium and compare them to earlier results. We also present the resistivity of lanthanum-nickel alloys (up to 60 at. % nickel) and of cerium-nickel alloys (up to 55 at. % nickel).

A. Liquid lanthanum

The electrical resistivity of 99.99% pure liquid lanthanum has been represented in Fig. 1 together with other authors' results. Our value at the melting point is very near that of Krieg *et al.*²⁰ but in our opinion their measurements grow too fast with temperature. The measurements²¹ of Gaibulaev *et al.* are about 22 $\mu\Omega$ cm lower than ours but their temperature dependence seems to us

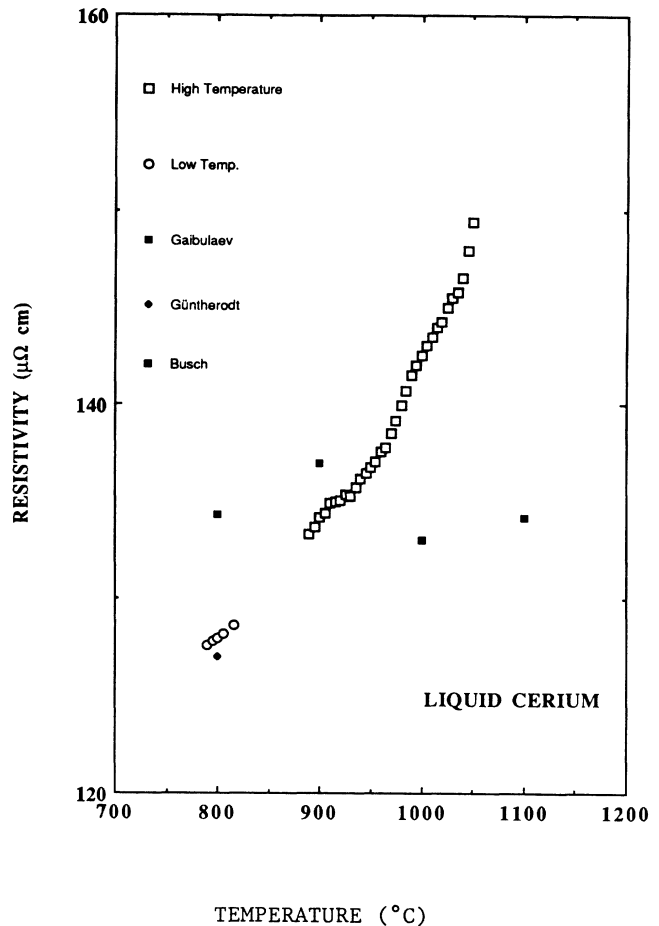


FIG. 2. Electrical resistivity of liquid cerium. The following have been represented: our low-temperature measurements; our high-temperature measurements; the values of Gaibulaev (Ref. 21); Busch *et al.* (Ref. 26); Güntherodt *et al.* (Ref. 22).

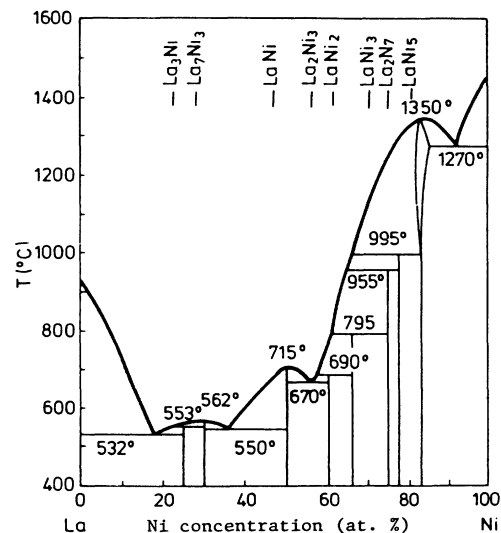


FIG. 3. Phase diagram of La-Ni (Ref. 21) after Buschow (1984) (Ref. 27).

more correct. The measurements,²²⁻²⁵ of Güntherodt *et al.* published in different papers are near our values; sometimes they are a little lower, sometimes a little higher. A time-dependent drift was superposed to the temperature dependence of the resistivity. It was estimated and corrected. An asymmetric error takes this drift into account. The admitted corrected values are 139.0 and 140.9 $\mu\Omega$ cm at, respectively, 950 and 1050 °C. This gives us a corrected temperature coefficient of 19 n Ω cm/°C (Gaibulaev, 24; Krieg, 136). Our corrected curve is given by

$$\rho = 0.01939T_c + 120.5 .$$

ρ is in $\mu\Omega$ cm and T_c in °C. It is consistent with Krieg's value at the melting point and with the last value of Güntherodt²⁵ at 1320 °C.

B. Liquid cerium

The electrical resistivity of 99.99% pure cerium is presented in Fig. 2 and compared to other authors'

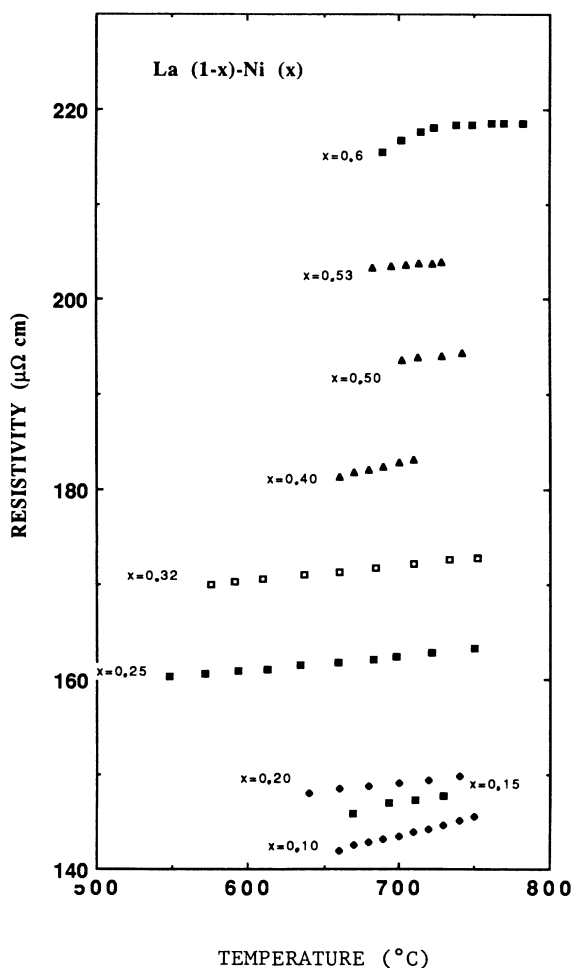


FIG. 4. Experimental electrical resistivity of liquid $\text{La}_{1-x}\text{Ni}_x$ alloys as a function of temperature.

values. Two experimental runs have been represented, one at high, the other at low temperatures only. The first run (crosses) presents a drift with time and the slope is too important; the second run (circles) is more accurate but limited in temperature. Our value at the melting point lies within 1% of Gaibulaev *et al.*²¹ and Güntherodt *et al.*^{22,24,25} and 8% of Busch *et al.*²⁶ These results may be considered as good with regard to the reactivity of these metals. We admit a resistivity given by our low-temperature run:

$$\rho = 0.0417T_c + 94.7 .$$

We believe that our value at the melting point is reliable but that perhaps the temperature coefficient is a little too high.

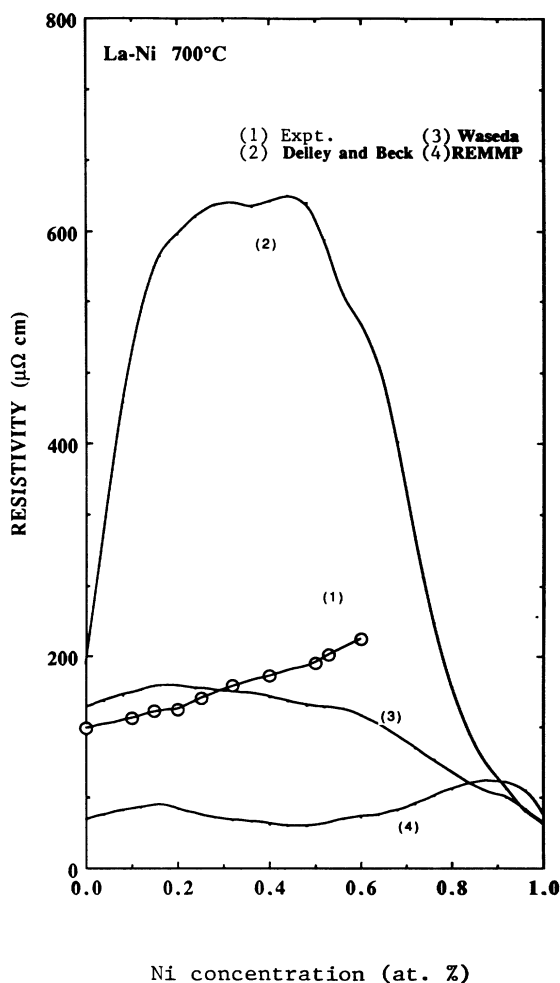


FIG. 5. Electrical resistivity of liquid La-Ni alloys as a function of nickel concentration at 700°C. Curve 1, experimental resistivity; curve 2, nonrenormalized phase shifts of Delley and Beck (Ref. 11) for lanthanum ($N_c = 0.91$) and of Dreirach *et al.* for nickel (Ref. 8); curve 3, phase shifts of Waseda (Ref. 8) for nickel and lanthanum ($N_c = Z = 3$); curve 4, rare-earth-metal model-potential results ($Z = 3$).

C. Liquid lanthanum-nickel alloys

The phase diagram of the La-Ni system is represented in Fig. 3 (Buschow²⁷). The electrical resistivity of eight La-Ni alloys has been reported as a function of temperature (Fig. 4) and concentration at 700°C (Fig. 5). The resistivity increases with nickel concentration, it reaches 219 $\mu\Omega$ cm at 60 at. % Ni, and is always growing with Ni concentration. This is probably due to the proximity of the compound La-Ni₅ with a liquidus temperature at 1350°C. With the electrical resistivity of liquid nickel being 85 $\mu\Omega$ cm (Kita *et al.*²⁸), it is evident that this alloy presents an important maximum. No drift with time has been observed at the measured temperatures (below 800°C).

D. Liquid cerium-nickel alloys

The phase diagram of the Ce-Ni system is represented in Fig. 6 (Hansen²⁹). The electrical resistivity of eight Ce-Ni alloys has been plotted as a function of temperature (Fig. 7) and composition at 700°C (Fig. 8). As for La-Ni, the resistivity grows with nickel concentration. The maximum seems, however, to be less pronounced.

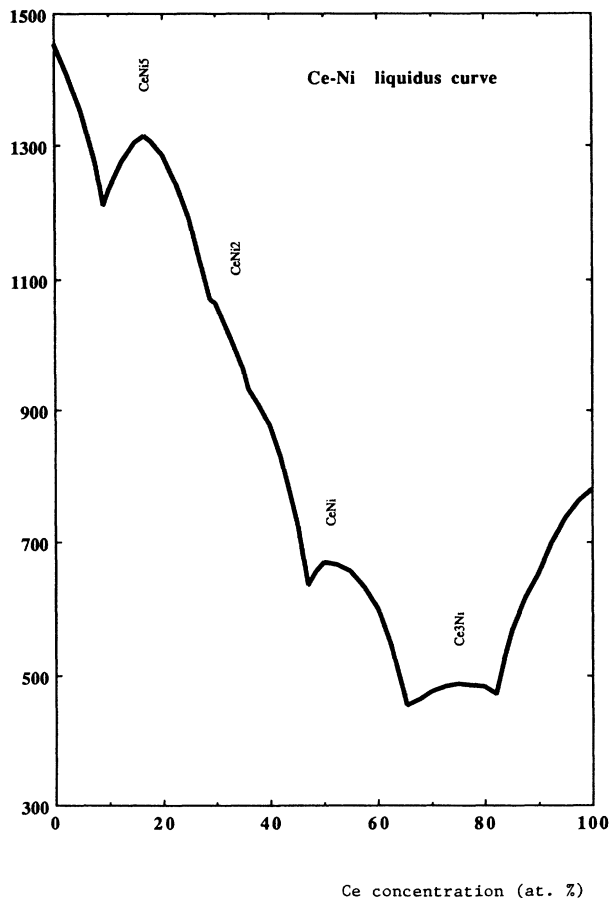


FIG. 6. Phase diagram of cerium-nickel after Hansen (Ref. 29).

We observed that for 27 at. % nickel the slope of the resistivity becomes negative. This phenomenon has not been observed with nickel-lanthanum alloys. The measurements have been performed by adding weighted quantities of metal in order to change the composition. We have determined by coming back to the same composition several days after that the resistivity drift is of about 1.4% by day. Ni-Ce raw measurements are represented in curve 1. The drift corrected values are represented in curve 2.

V. INTERPRETATION AND DISCUSSION

A. Pure rare-earth metals

The electrical properties of rare-earth metals have been interpreted in the framework of the "Ziman" formula with the REMMP potential and with the extended Faber-Ziman⁸ formula; the "pseudopotential form fac-

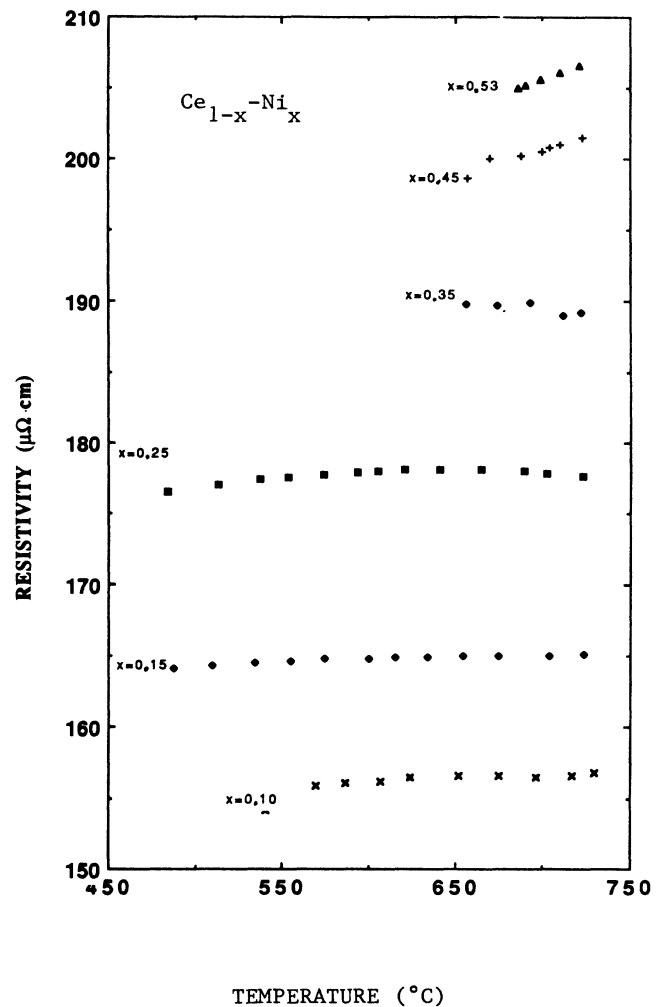


FIG. 7. Experimental electrical resistivity of Ce_{1-x}Ni_x alloys as a function of temperature.

tor" being simply replaced by the t matrix expressed as a function of phase shifts at the Fermi energy. Waseda *et al.*³⁰ have applied this technique to rare-earth metals and have computed the resistivity of liquid lanthanum and cerium. They admit, respectively, an electronic structure $(4f)^0(5d)^1(6s)^2$ and $(4f)^1(5d)^1(6s)^2$ with three valence electrons. The Fermi energy is calculated following a procedure proposed by Dreirach *et al.*⁸ as a function of the energy E_b of the bottom of the band relative to the muffin-tin zero. They obtain, respectively, 165 and 134 $\mu\Omega$ cm. However, Esposito *et al.*³¹ proposed a more consistent method to determine E_F without introducing E_b . It needs the definition of a new quantity, different from the valence (La and Ce are considered as trivalent elements): the number of "conduction electrons," N_c . Delley and Beck¹¹ used this method to compute consistently the resistivity of liquid lanthanum. Following the structure of the muffin-tin potential they obtain, respectively, $N_c=0.71, 0.92, 0.91$, and resistivities of 96,

133, and 158 $\mu\Omega$ cm with their renormalized phase shifts.

We computed the electrical resistivity of liquid lanthanum at the melting point, describing the structure with the hard-sphere structure factors or using the experimental structure factors tabulated by Waseda.⁹ The parameters and the expressions of the (REMMP) proposed by Upadhyaya *et al.*⁷ are given in their paper. With hard spheres we obtain, for liquid lanthanum, a resistivity of 45 $\mu\Omega$ cm with the REMMP; 293 $\mu\Omega$ cm with Delley phase shifts (and $N_c=0.91$), and 138 with Waseda's one ($N_c=Z=3$) at the melting point (920°C), to be compared to an experimental value of 138 $\mu\Omega$ cm. The influence of the structure is less important than that of the form factor. Indeed with Delley *et al.* nonrenormalized phase shifts we obtain 316 $\mu\Omega$ cm with the experimental structure factor. For liquid cerium the only available phase shifts are those given by Waseda⁹ with the nonrealistic assumption of three conduction electrons per atom. We obtain a resistivity of 114 $\mu\Omega$ cm at the melting point to be compared to an experimental value of 128 $\mu\Omega$ cm.

Ballentine *et al.*³² using a linear combination of atomic orbitals calculation of the valence band in liquid lanthanum showed that, although the diffusivity of s states is greater than the diffusivity of d states, the "much greater density of d states causes them to dominate the conductivity." In a hybridized s - d band model they obtain a resistivity of 151 $\mu\Omega$ cm. But in their conclusion they suggest that the "electrical conduction takes place via a kind of diffusion process for which the usual Boltzmann equation treatment is unjustifiable."

B. Alloys

The most important success of Ziman's formula has been the explanation of the negative temperature coefficient of the resistivity of liquid metals such as zinc in terms of the position of $2k_F$ compared to the position K_p of the main peak of the structure factor. This has been extended to alloys for which $2k_F$ moves from the left (monovalent metals), to the right (polyvalent metals) of the main peaks of the partial structure factors when the mean valency increases with the polyvalent metal concentration. It explains the negative temperature coefficient of noble-polyvalent alloys such as Cu-Sn (Busch *et al.*³³); transition-polyvalent alloys such as Mn-Sb, Mn-Sn, Mn-In, and Mn-Zn (Gasser^{16,34}); rare-earth-polyvalent alloys such as Ce-Sn (Güntherodt *et al.*²⁵).

Roughly it implies that the transition or rare-earth metals behave as monovalent ones ($N_c=1$). The fact that Ce-Ni presents a slightly negative temperature coefficient at 25 at. % Ni while La-Ni does not confirms experimentally the fact that the number N_c is probably different from one rare-earth metal to the other. Delley and Beck¹¹ calculated N_c values going from 0.71 (La) to 1.93 (Eu) but did not compute them for cerium. To our knowledge no quantitative theoretical result has yet been proposed for rare-earth alloys.

We interpreted the electrical properties of rare-earth metals in the framework of the Faber-Ziman formula with the REMMP potential and with the extended Faber-Ziman⁸ formula with the available phase shifts.

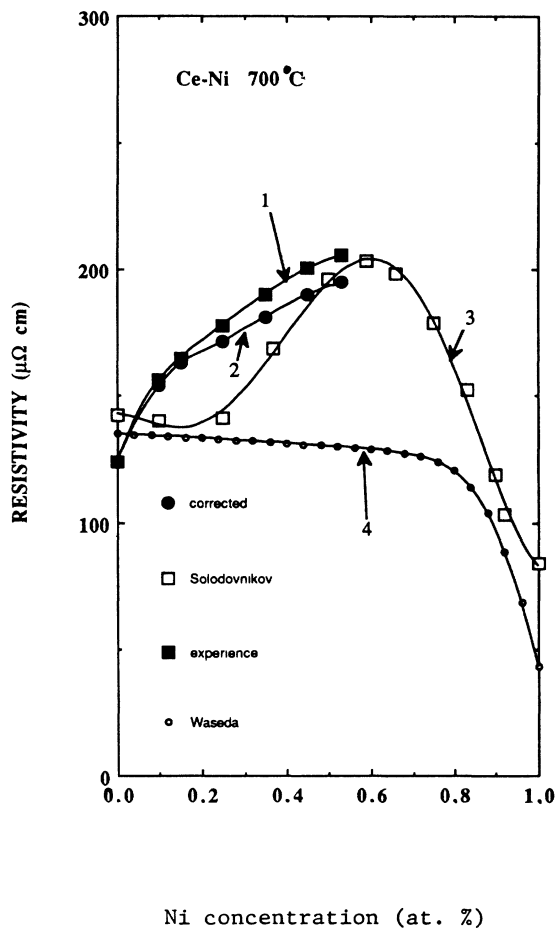


FIG. 8. Electrical resistivity of liquid Ce-Ni alloys as a function of concentration at 700°C. Curve 1 raw measurements; curve 2, drift corrected experimental curve; curve 3, Solodovnikov (Refs. 17 and 18) experimental curve; curve 4, calculated resistivity with Waseda phase shifts for nickel and cerium ($Z=3$).

1. Nickel-lanthanum alloys

The experimental (curve 1) and calculated (curves 2–4) electrical resistivities of Ni-La alloys as a function of concentration are represented in Fig. 5 (at 700°C). The REMMP form factor gives us a resistivity (curve 4) with a minimum at 50 at. % nickel (39 $\mu\Omega$ cm) while our measurements give 217 $\mu\Omega$ cm. This potential completely fails to describe the electronic properties if we use the valence 3 attributed to lanthanum. We tried to look at what is obtained with the same parameters if we crudely replace the valency $Z=3$ by a number of conduction electrons of 0.91 like the value given by Delley and Beck.¹¹

The results (not represented) present a maximum at 40 at. % Ni. The values are too high on the lanthanum rich side of the phase diagram. However, this result must only be considered as indicative, since the parameters of the potential must be recalculated with a correct number of conduction electrons.

We represent on curves 3 and 2 the t matrix results. Curve 2 is obtained with Delley *et al.*¹¹ nonrenormalized phase shifts for lanthanum and Dreirach *et al.*⁸ phase shifts for nickel; curve 3 is calculated with Waseda phase shifts³⁰ and a number of conduction electrons of 3 for lanthanum. The Waseda values give a better result for liquid lanthanum but this is probably fortuitous. Indeed, contrary to the experimental curve, the calculated resistivity is a monotonous decreasing curve from lanthanum to nickel. The nonrenormalized phase shifts of Delley give a value two times greater than their renormalized ones for pure lanthanum, but the maximum form of the experimental curve is reproduced. The maximum is located at 40 at. % Ni (like the REMMP) while the extrapolation of our experimental curve indicates that it seems to be near the compound composition Ni₅-La. It is evident that near the compound composition a hard-sphere description of the partial structure factors is no more correct. Above 200 $\mu\Omega$ cm the mean free path is of the order of the interatomic distance and multiple scattering can no more be neglected.

2. Nickel-cerium alloys

The Solodovnikov *et al.*^{17,18} measurements have been performed with an electrodeless method in a conducting tantalum container between 1100 and 1600°C. Their concentration curve at 1550°C presents a minimum at 20 at. % Ni which we do not observe at 700°C. A linear extrapolation of our measurements at 15 and 25 at. % Ni, with our slight positive temperature coefficient, gives us values greater than the Solodovnikov *et al.*^{17,18} ones, from about 25 $\mu\Omega$ cm. Solodovnikov *et al.*^{17,18} interpreted their experimental results with the Faber-Ziman formula. However, their calculations differ from ours from several points of view. Their alloy partial structure factors are the pure liquid metals (Ashcroft and Lekner³⁵) ones, while the $a_{12}(q)$ structure factor is the concentration weighted mean value of the pure liquid metal structure factors. In our calculation we used Ashcroft-Langreth¹³ partial structure factors.

A second important difference occurs in the expression of $t_i(q)$, where they used the pure-metal atomic volume as

a normalization factor, while we renormalized $t_i(q)$ on the atomic volume of the alloy.

Other differences occur in the values of the parameters such as the valency, the effective mass, and the phase shifts. We can compare the calculated curve 1 of Fig. 3 of Solodovnikov *et al.*¹⁷ with our calculated curve 3 of Fig. 8. Our curve is a monotonously decreasing function with nickel concentration, while Solodovnikov *et al.* found a double maximum curve. The most important difference occurs in the Solodovnikov *et al.*¹⁸ hypothesis of a variable number of conduction electrons. This number produced by cerium on alloying with nickel (curve 3 of Fig. 3 of Ref. 1) has been fitted on the alloy resistivity.

Their discussion is interesting, but it seems to us daring to conclude on a variable number of conduction electrons with their crude hypothesis of alloy structure factors identical to the pure-metal ones and without renormalization of the atomic volume which can be three times greater. In Fig. 6 we have represented the raw experimental, the drift corrected experimental, the experimental, the experimental values of Solodovnikov *et al.*, and the calculated resistivity of liquid Ni-Ce as a function of concentration at 700°C. As for lanthanum alloys, the valency is taken equal to 3. The calculated curve is a monotonous decreasing one and cannot explain the experimental values.

VI. CONCLUSION

In this paper we present resistivity measurements on transition-metal-rare-earth liquid alloys. The concentration curve shows the existence of a maximum in the transition-metal rich side of the phase diagram. For high resistivity alloys, the temperature coefficient is always positive confirming the Mooij³⁶ empirical rule.

It has been postulated in earlier work that transition metals behave as monovalent ones. Our measurements prove experimentally that lanthanum and cerium do not behave as trivalent nor divalent metals. If it were the case, we should observe negative temperature coefficients in a large interval of concentration.

Calculations have been performed both with pseudopotential and t -matrix formalisms. Evidently, the single-site scattering approach cannot be used for nickel-rich alloys where multiple scattering cannot be neglected. Even for rare-earth-rich alloys the extended Faber-Ziman formalism calculations cannot be considered as good. Indeed, the pseudopotential form factor (and k_F) has been calculated with a valency of 3 which is not realistic for rare-earth metals. The Waseda phase shifts (with $Z=3$) give (fortuitously?) good results for pure rare-earth metals but cannot explain the alloy results.

The nonrenormalized phase shifts of Delley and Beck give too high values and a maximum in the lanthanum-rich side of the phase diagram. Their more realistic renormalized phase shifts, giving a good result for pure lanthanum, are not available.

The concentration independence of phase shifts produces a strong maximum as has been shown by Gasser for manganese-polyvalent alloys.¹⁶ The energy depen-

dence must be taken into account by alloying.

Much theoretical work remains to be done in order to interpret the experimental resistivities: The pseudopotential parameters must be recalculated with a lower valen-

cy; the renormalized phase shifts must be made available; the energy dependence of the phase shifts with composition must be taken into account, even crudely; multiple scattering cannot be neglected.

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