JOURNAL OF MATERIALS SCIENCE 21 (1986) 2767–2770

Remarks on the use of Boltzmann's equation for electrical conduction calculations in metal matrix and *in situ* composites

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The Boltzmann equation and its solutions are cental to the development of microscopic models describing the longitudinal and transverse electrical conductivity of metal matrix and *in situ* composites. Such solutions are needed to describe electron and phonon scattering and transport phenomena in the matrix due to the presence of a second filamentary phase, and to describe electrical conductivity at cryogenic and higher temperatures. In this paper, we derive solutions to the Boltzmann equation in the relaxation time approximation in cylindrical co-ordinates. It is shown that one solution for the electric field parallel to the fibre direction leads to an expression for composite conductivity at cryogenic and higher temperatures. We also present a solution for the case in which the electric field is normal to the fibre direction.

1. Introduction

A number of experimental studies on the electrical conductivity of metal matrix and *in situ* composite materials have been reported [1–6]. In these studies, experimental results are discusssed and related to conduction models. These models are either modified forms of the rule of mixture or simple equations based on Dingle's [7] asymptotic solution for electrical conduction in thin wires and thin films when the reinforcing filaments are either much larger or much smaller than the bulk electron mean free path. To some extent, these models provide a simple theoretical explanation of the observed phenomena, but because of their simplicity, fail to provide a satisfactory insight into the phenomena of low-temperature conduction (resistivity) in metal matrix and *in situ* composites. Moreover, these models are limited to the experiments under discussion and, consequently, are inadequate for the prediction of the electrical behaviour of composites at low temperatures in general.

A general theory of composite conduction at cryogenic and higher temperatures was developed by Roig and Schoutens [8]. This theory is founded on a solution of the Boltzmann equations and applied, after numerical integration, to the electrical conduction of a metal matrix composite (MMC) in a direction parallel to the reinforcing fibres. A similar approach is now being developed by Roig and Schoutens [9] for the electrical conduction of MMCs in a direction transverse to the reinforcing fibres. The Boltzmann equations and its solutions were also applied to describe the resistivity phenomena of thin reaction regions and thin-walled tubes around a non-conducting fibre [10].

In these developments, the Boltzmann equation and its solutions are central to an understanding of low-temperature electrical conduction phenomena in metal matrix and *in situ* composites. Solutions to the Boltzmann equation are needed to describe electron and phonon scattering and transport phenomena in the matrix as a result of their interaction with fibre surfaces.

In describing longitudinal composite electrical conduction at low temperature [8], we dealt with the problem of electron transport in MMC materials by solving the linearized Boltzmann equation with a small electric field directed along the axis of the fibres. The mean free path for electron scattering from the fibre surfaces was assumed to be no greater than half the average fibre separation distances. Thus, there was essentially no overlap between scattering regions for adjacent fibres. Consequently, the problem reduced to that of finding the scattering from the external surface of a cylindrical surface. For this purpose, we applied the appropriate boundary conditions at the fibre surface to the general solution of the Boltzmann equation with cylindrical symmetry found by Dingle [7]. The same general solution was used to calculate the electrical conductivity of thin-walled tubes and the boundary conditions were applied to the surfaces of two coaxial cylinders [10].

Dingle [7] solved the Boltzmann equation with cylindrical symmetry using an indirect approach: first, he found the general solution in rectangular co-ordinates, and then selected the solutions with the appropriate symmetry. In this paper, we solve the Boltzmann equation directly in cylindrical co-ordinates. The method is general and straightfoward. First, we find the general solution when there is cylindrical symmetry, and then, we find the general solution when

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there is no cylindrical symmetry. The latter solution is of interest when dealing with the problem of overlapping scattering regions mentioned above and when the electric field is transverse to the fibre axis.

2. The solution of the Boltzmann equation with cylindrical symmetry

The linearized Boltzmann equation in rectangular co-ordinates, in the relaxation time approximation, and with small applied electric field $\bar{E}$ is

$$\bar{v} \cdot \nabla_{\bar{r}} F^1(\bar{r}, \bar{v}) + \frac{F^1(\bar{r}, \bar{v})}{\tau} = \frac{e\bar{E}}{m^*} \cdot \nabla_{\bar{v}} F^0(v) \quad (1)$$

where e is the absolute value of the electronic charge and m^* is its effective mass, τ is the relaxation time for scattering, $\bar{v} = \bar{v}(v_x, v_y, v_z)$ is the electron velocity, $\bar{r}(x, y, z)$ is the electron position, and F^1 is the change in the equilibrium distribution function F^0 when a small electric field is applied.

If we consider a unidirectional fibre reinforced metal with $\bar{E}$ directed along the axis of the fibres, Equation 1 becomes

$$v_x \frac{\partial F^1}{\partial x} + v_y \frac{\partial F^1}{\partial y} + \frac{F^1}{\tau} = \frac{eE}{m^*} \frac{\partial F^0}{\partial v_z} \quad (2)$$

where the z-axis is parallel to the electric field. Taking cylindrical co-ordinates $x = r\cos\theta$, $y = r\sin\theta$, and $z = z$, we obtain for the velocity

$$v_x = v_r \cos\theta - v_\theta \sin\theta \quad (3)$$

$$v_y = v_r \sin\theta + v_\theta \cos\theta \quad (4)$$

$$v_z = v_z \quad (5)$$

Now, when the problem has cylindrical symmetry, F^1 does not depend on the angle θ and the two partial derivatives in x and y become

$$\frac{\partial}{\partial x} = \cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r}\left(v_\theta \frac{\partial}{\partial v_r} - v_r \frac{\partial}{\partial v_\theta}\right) \quad (6)$$

$$\frac{\partial}{\partial y} = \sin\theta \frac{\partial}{\partial r} + \frac{\cos\theta}{r}\left(v_\theta \frac{\partial}{\partial v_r} - v_r \frac{\partial}{\partial v_\theta}\right) \quad (7)$$

Consequently, Equation 2 transforms into

$$v_r \frac{\partial F^1}{\partial r} + \frac{v_\theta^2}{r}\frac{\partial F^1}{\partial v_r} - \frac{v_\theta v_r}{r}\frac{\partial F^1}{\partial v_\theta} + \frac{F^1}{\tau} = \frac{eE}{m^*}\frac{\partial F^0}{\partial v_z} \quad (8)$$

Equation 8 can be solved directly using general methods from the theory of quasilinear first order partial differential equations [11]. The characteristic system associated with Equation 8 is

$$\frac{dr}{v_r} = \frac{r dv_r}{v_\theta^2} = -\frac{r dv_\theta}{v_\theta v_r} = \frac{dF^1}{A - F^1/\tau} \quad (9)$$

where

$$A = \frac{eE}{m^*}\frac{\partial F^0(v)}{\partial v_z} = \frac{eE}{m^*}\frac{v_z}{v}\frac{\partial F^0(v)}{\delta v} \quad (10)$$

$$v = (v_r^2 + v_\theta^2 + v_z^2)^{1/2} \quad (11)$$

To find the general solution of Equation 8, we need to find first three independent integrals of the system of Equation 9. These are obtained as follows from

$$\frac{dr}{v_r} = -\frac{r dv_\theta}{v_\theta v_r} \quad (12)$$

it follows immediately that

$$r v_\theta = \text{constant} \equiv \alpha \quad (13)$$

and from

$$\frac{r dv_r}{v_\theta^2} = -\frac{r dv_\theta}{v_\theta v_r}$$

the results

$$v_r^2 + v_\theta^2 = \text{constant} \equiv \beta \quad (14)$$

Next, we consider

$$\frac{dr}{v_r} = \frac{r dv_r}{v_\theta^2} = \frac{dF^1}{A - F^1/\tau} \quad (15)$$

or

$$\frac{v_r dr + r dv_r}{v_r^2 + v_\theta^2} = \frac{dF^1}{A - F^1/\tau} \quad (16)$$

Now, A is of the form $v_z g(v) = v_z g[(v_r^2 + v_\theta^2 + v_z^2)^{1/2}]$, which, when introduced into Equation 16 together with Equation 14, gives

$$\frac{d(rv_r)}{\beta} = \frac{dF^1}{v_z g[(\beta + v_z^2)^{1/2}] - (F^1/\tau)} \quad (17)$$

and since v_z is just a parameter, Equation 17 can be integrated to give

$$\left\{v_z g[(\beta + v_z^2)^{1/2}] - \frac{F^1}{\tau}\right\} \exp\left(\frac{rv_r}{\tau\beta}\right) = \text{constant} \equiv \gamma \quad (18)$$

and replacing β by its definition given above, we obtain the integral

$$\left(A - \frac{F^1}{\tau}\right) \exp\left[\frac{rv_r}{(v_r^2 + v_\theta^2)\tau}\right] = \text{constant} \equiv \gamma \quad (19)$$

The general solution of Equation 8 is now obtained by setting an arbitrary relationship between the three integration constants α, β, and γ, or $F(\alpha, \beta, \gamma) = 0$. Using the integrals given by Equations 13, 14 and 19 to eliminate these constants, we obtain

$$F\left\{rv_\theta, v_r^2 + v_\theta^2, \left(A - \frac{F^1}{\tau}\right)\exp\left[\frac{rv_r}{(v_r^2 + v_\theta^2)\tau}\right]\right\} = 0 \quad (20)$$

which is the general solution to Equation 8. Equation 20 can be rewritten in the form

$$\left(A - \frac{F^1}{\tau}\right)\exp\left[\frac{rv_r}{(v_r^2 + v_\theta^2)\tau}\right] = \Phi(rv_\theta, v_r^2 + v_\theta^2) \quad (21)$$

where Φ is an arbitrary function. Letting $\Phi = Af$ with f arbitrary, the general solution, Equation 21, becomes

$$F^1 = \frac{eE\tau}{m^*}\frac{\partial F^0}{\partial v_z} \times \left[1 - f(rv_\theta, v_r^2 + v_\theta^2)\exp\left(-\frac{1}{\tau}\frac{rv_r}{v_r^2 + v_\theta^2}\right)\right] \quad (22)$$

This is the same solution found by Dingle [7] using an indirect method. The function f is determined from the boundary conditions of the problem.

3. Applications of the general solutions

We consider two cases: Case A in which the electric field is directed along the axis of the fibre (z-axis), and Case B in which the electric field is transverse to the fibre axis. In both cases, the distribution function depends on the angle θ and all other variables. Therefore, the partial derivatives in x and y become

$$\frac{\partial}{\partial x} = \cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r}\left(\frac{\partial}{\partial\theta} + v_\theta \frac{\partial}{\partial v_r} - v_r \frac{\partial}{\partial v_\theta}\right) \tag{23}$$

$$\frac{\partial}{\partial y} = \sin\theta \frac{\partial}{\partial r} + \frac{\cos\theta}{r}\left(\frac{\partial}{\partial\theta} + v_\theta \frac{\partial}{\partial v_r} - v_r \frac{\partial}{\partial v_\theta}\right) \tag{24}$$

which are now used to construct solutions for each case.

3.1. Case A: parallel electric field

When the electric field is parallel to the axis of the fibres, the Boltzmann equation is

$$v_r \frac{\partial F^1}{\partial r} + \frac{v_\theta^2}{r}\frac{\partial F^1}{\partial v_r} - \frac{v_r v_\theta}{r}\frac{\partial F^1}{\partial v_\theta} + \frac{v_\theta}{r}\frac{\partial F^1}{\partial\theta} + \frac{F^1}{\tau} = \frac{eE}{m^*}\frac{\partial F^0}{\partial v_z} \tag{25}$$

and the characteristic system is

$$\frac{dv_r}{v_r} = \frac{r dv_r}{v_\theta^2} = -\frac{r dv_\theta}{v_\theta v_r} = \frac{r d\theta}{v_\theta} = \frac{dF^1}{A - F^1/\tau} \tag{26}$$

The general solution of Equation 25 requires four independent integrals of Equation 26. Three of these integrals are Equations 13, 14 and 19, and the fourth integral is obtained from

$$-\frac{r dv_\theta}{v_\theta v_r} = \frac{r d\theta}{v_\theta} \tag{27}$$

Introducing $v_r = +(\beta - v_\theta^2)^{1/2}$, where Equation 14 with the positive root was used, Equation 27 becomes

$$-\frac{dv_\theta}{(\beta - v_\theta^2)^{1/2}} = d\theta \tag{28}$$

which integrates to

$$\theta + \sin^{-1}\left[\frac{v_\theta}{(v_r^2 + v_\theta^2)^{1/2}}\right] = \text{constant} \equiv \delta \tag{29}$$

It can be easily verified that the negative sign for the square root of v_r does not result in a solution to the Boltzmann equation. Proceeding as in Section 2, we obtain the general solution

$$F^1 = \frac{eE\tau}{m^*}\frac{\partial F^0}{\partial v_z}\left\{1 - f(rv_\theta, v_r^2 + v_\theta^2, \theta + \varphi) \times \exp\left[-\frac{1}{\tau}\left(\frac{rv_r}{v_r^2 + v_\theta^2}\right)\right]\right\} \tag{30}$$

with

$$\varphi = \sin^{-1}\left[\frac{v_\theta}{(v_r^2 + v_\theta^2)^{1/2}}\right] \tag{31}$$

This solution can be used to find the electrical conductivity when the scattering regions from adjacent fibres overlap. The solution without overlap in scattering regions was used to calculate the electrical conductivity for an MMC with the electrical field parallel to the fibre axis. This led to the following equation [8]

$$\frac{\sigma}{\sigma_0} = 1 - (1 - p)\frac{6a^2}{A_c}\int_1^{(1+2/k)} x dx \int_0^{\pi/2} \cos^2\theta \sin\theta\, d\theta \times \int_0^{\sin^{-1}(1/x)} \exp\{-k[x\cos\varphi - (1 - x^2\sin^2\varphi)^{1/2}]/(2\sin\theta)\}\, d\varphi \tag{32}$$

where $x = r/a$; a is the fibre radius; $k = 2a/\Lambda_0$, where Λ_0 is the electron scattering mean free path; θ and φ are position angles; A_c is the cross-sectional area of the region of interest, in this case, a square cell with a fibre in each corner; p is the fibre surface reflection coefficient; σ is the conductivity within the cell altered by fibre surface scattering; and σ_0 is the bulk conductivity. Equation 32 was integrated numerically [8], resulting in a linear relationship between the value of the integrals and k. Assuming that the fibre surfaces are rough relative to the electron scattering mean free path, we set $p = 0$, and using the definition of the fibre volume fraction for the square cell of interest, we obtained the following equation for the composite electrical resistance (conductivity) along the fibre

$$\varrho_c(T) = \varrho_0 \times \left\{(1 - V_f)\left[1 - 21.23\left(\frac{V_f}{1 - V_f}\right)^2 (3 + T)T^{-3.08}\right]\right\}^{-1} \tag{33}$$

This equation was derived on the assumption that there is a simple linear relationship between k and temperature. Therefore, this equation shows a sharp rise in electric resistivity of a composite at very low temperatures [8]. At temperatures above about 100 K, it predicts that $\varrho_c(T) = \varrho_0(1 - V_f)^{-1}$, in agreement with experimental data [12]. Note that the assumption of $p = 0$ is not correct for *in situ* composites because it has been observed that the surfaces of such *in situ* filaments are quite smooth and, hence, $p \simeq 0$ to 0.5 [1, 2].

3.2. Case B: transverse electric field

When the electrical field is transverse to the fibres, the right-hand side of Equation 25 is given by

$$\frac{eE}{m^*}\frac{\partial F^0}{\partial v_y} = \frac{eE}{m^*}\frac{v_y}{v}\frac{\partial F^0}{\partial v} = v_y h(v) \tag{34}$$

where we have chosen the y-axis parallel to the electric field direction and perpendicular to the fibre direction. Equation 4 gives v_y in terms of v_r and v_θ, and v is given by Equation 11. Thus, the Boltzmann equation becomes

$$v_r \frac{\partial F^1}{\partial r} + \frac{v_\theta^2}{r}\frac{\partial F^1}{\partial v_r} - \frac{v_r v_\theta}{r}\frac{\partial F^1}{\partial v_\theta} + \frac{v_\theta}{r}\frac{\partial F^1}{\partial\theta} + \frac{F^1}{\tau} = (v_r \sin\theta + v_\theta\cos\theta)h(v) \tag{35}$$

The characteristic system has Equations 13, 14 and 29 as integrals, and the fourth integral is obtained from

$$\frac{\mathrm{d}r}{v_r} = \frac{r\mathrm{d}v_r}{v_\theta^2} = \frac{\mathrm{d}F^1}{(v_r \sin\theta + v_\theta \cos\theta)h(v) - F^1/\tau}$$

or

$$\frac{\mathrm{d}(rv_r)}{v_r^2 + v_\theta^2} = \frac{\mathrm{d}F^1}{(v_r \sin\theta + v_\theta \cos\theta)h(v) - F^1/\tau} \quad (36)$$

Now, $v_r \sin\theta + v_\theta \cos\theta = (v_r^2 + v_\theta^2)^{1/2} (\cos\varphi \sin\theta + \sin\varphi \cos\theta) = (v_r^2 + v_\theta^2)^{1/2} \sin(\theta + \varphi)$, where $\cos\varphi = v_r/(v_r^2 + v_\theta^2)^{1/2}$ and $\sin\varphi = v_\theta/(v_r^2 + v_\theta^2)^{1/2}$. Then, substituting into Equation 36 and inserting the integrals 14 and 29, there results

$$\frac{\mathrm{d}(rv_r)}{\beta} = \frac{\mathrm{d}F^1}{\beta^{1/2}h[(v_z^2 + \beta)^{1/2}] \sin\delta - F^1/\tau} \quad (37)$$

which, when integrated, gives

$$\left\{\beta^{1/2}h\left[(v_z^2 + \beta)^{1/2}\right] \sin\delta - \frac{F^1}{\tau}\right\} \times \exp\left(\frac{rv_r}{\tau\beta}\right) = \text{constant} = \varepsilon \quad (38)$$

and since $\beta = v_r^2 + v_\theta^2$ and $\delta = \theta + \varphi$, we finally obtain the fourth integral, or

$$\left[\sin(\theta + \varphi)(v_r^2 + v_\theta^2)^{1/2}h(v) - \frac{F^1}{\tau}\right] \times \exp\left[\frac{rv_r}{\tau(v_r^2 + v_\theta^2)}\right] = \varepsilon \quad (39)$$

But, $\sin(\theta + \varphi)(v_r^2 + v_\theta^2)^{1/2}h(v) = (eE/m^*)\partial F^0/\partial v_y$; then, the general solution in transverse field can be written as

$$\left(\frac{eE}{m^*}\frac{\partial F^0}{\partial v_y} - \frac{F^1}{\tau}\right) \exp\left[\frac{rv_r}{\tau(v_r^2 + v_\theta^2)}\right] = \Phi(rv_\theta, v_r^2 + v_\theta^2, \theta + \varphi) \quad (40)$$

where Φ is an arbitrary function, and when solving for F^1, we obtain

$$F^1 = \frac{eE\tau}{m^*}\frac{\partial F^0}{\partial v_y} - \tau\Phi(rv_\theta, v_r^2 + v_\theta^2, \theta + \varphi) \times \exp\left[-\frac{rv_r}{\tau(v_r^2 + v_\theta^2)}\right] \quad (41)$$

Using the fact that $\partial F^0/\partial v_y = (v_y/v)\partial F^0 \partial v$, and recognizing that $v = (v_r^2 + v_\theta^2 + v_z^2)^{1/2}$ and $v_y = v_r \sin\theta + v_\theta \cos\theta$, Equation 41 becomes

$$F^1 = \frac{eE\tau}{m^*}\frac{\partial F^0}{\partial v}\left\{1 - \frac{1}{v_r \sin\theta + v_\theta \cos\theta} \times f(rv_\theta, v_r^2 + v_\theta^2, \theta + \varphi) \exp\left[-\frac{rv_r}{\tau(v_r^2 + v_\theta^2)}\right]\right\} \quad (42)$$

where

$$f(rv_\theta, v_r^2 + v_\theta^2, \theta + \psi) = \left(\frac{eE}{m^*}\frac{1}{v}\frac{\partial F^0}{\partial v}\right)^{-1} \times \Phi(rv_\theta, v_r^2 + v_\theta^2, \theta + \varphi) \quad (43)$$

where f is an arbitrary function to be determined from the boundary conditions. Equation 42 is the general solution of the Boltzmann equation in a transverse electric field. This solution can be used to calculate the transverse resistance of metal matrix and *in situ* composite materials. Note that in the absence of boundary surfaces, the solution given by Equation 42 reduces to

$$F^1 = \frac{eE\tau}{m^*}\frac{\partial F^0}{\partial v} \quad (44)$$

which is the bulk solution when the electrical field is along the y-axis.

4. Conclusions

The Boltzmann equation in the relaxation time approximation has been solved directly using cylindrical co-ordinates. It is found that the only difference between the general solution when there is no cylindrical symmetry and the general solution when there is cylindrical symmetry is the addition of an angular variable to the arbitrary function that appears in the latter solution. This angular variable consists of the sum of two angles: one is the angle θ defined by the cylindrical co-ordinates, and the other is the angle ϕ defined by the radial and tangential components of the electron velocity. The general solution can be used to calculate the electrical resistivity of metal matrix and *in situ* composites for an electrical field along the fibre direction when the scattering regions of adjacent fibres overlap, and to calculate the electrical resistivity of the composites when the electrical field is normal to the fibre direction. We have presented such a solution for the electrical resistivity of MMCs when the electric field is parallel to the fibres and in the absence of overlapping scattering regions.

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Received 21 August and accepted 3 October 1985