SOLUTION FOR QUIZ #1 6.732 10/16/98

60 Points

1. (a). (10 points)

$(0.75, 0.75, 0)\frac{\pi}{a}$

$$n = \frac{1}{4\pi^3}\int d^3k = \frac{1}{4\pi^3}\int dk_1 \int dk_2 \int dk_3$$

$$E = \frac{\hbar^2}{2}\left(\frac{k_1^2}{m_1} + \frac{k_2^2}{m_2} + \frac{k_3^2}{m_3}\right)$$

let $k_\alpha' = \sqrt{\frac{m_0}{m_\alpha}}\, k_\alpha$, $\Rightarrow E = \frac{\hbar^2}{2m_0}(k')^2$.

$$\Rightarrow n = \frac{1}{4\pi^3}\cdot 4\pi\cdot\sqrt{2}\cdot\left(m_1 m_2 m_3/m_0^3\right)^{1/2}\cdot\left(\frac{m_0}{\hbar^2}\right)^{3/2}\cdot\int_0^{E_F}\sqrt{E}\cdot dE, \quad \begin{cases} m_1 = m_0 \\ m_2 = m_0/3 \\ m_3 = m_0/9 \end{cases}$$

$$= \frac{1}{3\pi^2}\cdot\left(\frac{2m_0}{2\hbar^2}\right)^{3/2}\cdot E_F^{3/2},$$

$$\Rightarrow E_F = \frac{3\hbar^2}{2m_0}\cdot\left(3n\pi^2\right)^{3/2};$$

Shortest k_F from the smallest mass $\rightarrow$

$$E_F = \frac{3\hbar^2}{2m_0}\cdot\left(3n\pi^2\right)^{3/2} = \frac{\hbar^2}{2}\cdot\left(\cancelto{0}{\frac{k_1^2}{m_1}} + \cancelto{0}{\frac{k_2^2}{m_2}} + \frac{k_3^2}{m_3}\right),$$

$$\Rightarrow K_{F\,min} = k_3 = \frac{\sqrt{3}}{3}\left(3n\pi^2\right)^{1/3};$$

(b). (5 points) in (111) direction, $k_1 = k_2 = k_3 = k$,

$$\Rightarrow \frac{\hbar^2 k^2}{2}\cdot\left(\frac{1}{m_1} + \frac{1}{m_2} + \frac{1}{m_3}\right) = E_F, \quad \Rightarrow k = \sqrt{\frac{2E_F}{\hbar^2\cdot\left(\frac{1}{m_1}+\frac{1}{m_2}+\frac{1}{m_3}\right)}}$$

$$\Rightarrow K_F(111) = \sqrt{3}\,k = \sqrt{27/13}\;K_{F\,min};$$

(5 points) (c). There're 12 equivalent electron ellipsoidal pockets:

$(110), (1\bar{1}0), (\bar{1}10), (\bar{1}\bar{1}0)$;

$(011), (0\bar{1}1), (01\bar{1}), (0\bar{1}\bar{1})$;

$(101), (10\bar{1}), (\bar{1}01), (\bar{1}0\bar{1})$;

(5 points) (d). For electrons,

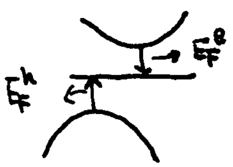
$$g(E)\,dE = \frac{1}{2\pi^2}\cdot\sqrt{m_1 m_2 m_3}\cdot\left(\frac{2}{\hbar^2}\right)^{3/2}\cdot\sqrt{E}\cdot dE, \quad 12 \text{ pockets},$$

$\Rightarrow$ DOS $= 12 * g(E)$;

(5 pts) (e). For holes, since they are all spherical pockets,

$$g_i(E) = \frac{1}{2\pi^2}\cdot\left(\frac{2m_{ih}}{\hbar^2}\right)^{3/2}\cdot\sqrt{E}\cdot dE,$$ where m_{ih} = masses for 3 different hole pockets;

(10 pts) (f). at T, for electron pockets,



$$n_e = 12\times\frac{1}{4\pi^3}\cdot\int f_0(E)\,dk^3,\qquad \begin{cases} f_0(E) = \dfrac{1}{e^{(E-E_F^e)/kT}+1} \cong e^{(-E-|E_F^e|)/kT} \\ E = \dfrac{\hbar^2}{2}\cdot\left(\dfrac{k_1^2}{m_1}+\dfrac{k_2^2}{m_2}+\dfrac{k_3^2}{m_3}\right) \end{cases},$$

$$\Rightarrow n_e = 12\times\frac{1}{2\pi^2}\cdot\sqrt{m_1 m_2 m_3}\cdot\left(\frac{2}{\hbar^2}\right)^{3/2}\cdot e^{-|E_F^e|/kT}\cdot\int_0^\infty e^{-E/kT}\cdot\sqrt{E}\cdot dE$$

$$= \frac{8}{\sqrt{3}}\cdot\left(\frac{m_0 kT}{2\pi\hbar^2}\right)^{3/2}\cdot e^{-|E_F^e|/kT}; \qquad (1)$$

For the holes, (ignore soh here since $e^{-0.1eV/kT} \ll 1$).

$$n_h = n_{hh} + n_{lh} = \frac{1}{2\pi^2}\cdot\left(\frac{2m_{hh}}{\hbar^2}\right)^{3/2}\cdot e^{-|E_F^h|/kT}\cdot\int_0^\infty dE\cdot e^{-E/kT}\cdot\sqrt{E}\cdot dE + \text{l.h. term}, \quad (2)$$

For an intrinsic semiconductor, $n_e = n_h$, and $|E_F^e| + |E_F^h| = E_g$,

equate (1) and (2), $\Rightarrow$ $|E_F^e| = \frac{1}{2}E_g - \frac{1}{2}kT \cdot \ln\left(\frac{m_{hh}^{3/2} + m_{lh}^{3/2}}{\sqrt{m_1 m_2 m_3}}\right)$

10 pts

(f). Let n be electron density for a single pocket,

$12n = n_{lh} + n_{hh}$, and $n_{ih} \propto m_{ih}^{3/2}$, $\Rightarrow$

$n_{hh} : n_{lh} : n = 1 : \left(\frac{1}{3}\right)^{3/2} : \frac{12}{\left(1+\frac{1}{3\sqrt{3}}\right)}$;

Since holes are spherical, contributions from holes are,

$$\sigma_h = \sigma_{hh} + \sigma_{lh} = \frac{n_{hh}e^2\tau}{m_{hh}} + \frac{n_{lh} \cdot e^2 \cdot \tau}{m_{lh}}$$

$$= \frac{e^2 \cdot \tau \cdot n}{m_0} \cdot 12 \cdot \frac{\left(1+\frac{1}{\sqrt{3}}\right)}{\left(1+\frac{1}{3\sqrt{3}}\right)} \cong 15.9 \cdot \left(\frac{ne^2\tau}{m_0}\right),$$

For the electron pockets, $\overleftrightarrow{\sigma} = \frac{ne^2\tau}{m_0} \cdot \begin{pmatrix} 1 & & 0 \\ & 3 & \\ 0 & & 9 \end{pmatrix}$; and we

consider only $\vec{E}$ in (110) direction:

By symmetry, the 12 electron pockets can be divided into

3 groups, A: (110) $(\bar{1}\bar{1}0)$ $(1\bar{1}0)$ $(\bar{1}10)$; B: (101) $(\bar{1}0\bar{1})$ $(\bar{1}01)$ $(10\bar{1})$; and

C: (011) $(0\bar{1}1)$ $(01\bar{1})$ $(0\bar{1}\bar{1})$;

Contributions from each pocket belonging to the same group will be the same. Also, for $\vec{E}(110)$, group B and C are symmetric, and give same contribution to σ.

So, for (110) pocket, $R_{110} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & -1 \end{pmatrix}$, $R_{110}^{-1} = R_{110}$,

$$\Rightarrow \overleftrightarrow{\sigma}_{lab} = R\, \overleftrightarrow{\sigma}_{crystal}\, R^{-1} = \frac{ne^2\tau}{m_0} \cdot \begin{pmatrix} 2 & -1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 9 \end{pmatrix},$$

$$\Rightarrow \vec{j} = \overleftrightarrow{\sigma}_{lab} \cdot \vec{E} = \frac{ne^2\tau}{m_0} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} E,$$

$$\Rightarrow \sigma_{110} = \frac{ne^2\tau}{m_0};$$

For other pockets, pick a particular one, (011),

$$R_{011} = \begin{pmatrix} 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \quad R_{011}^{-1} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} \\ 1 & 0 & 0 \end{pmatrix}, \quad \Rightarrow \overleftrightarrow{\sigma}_{lab} = \frac{ne^2\tau}{m_0} \cdot \begin{pmatrix} 9 & 0 & 0 \\ 0 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix},$$

$$\Rightarrow \vec{j} = \overleftrightarrow{\sigma}_{lab} \cdot \vec{E} = \frac{ne^2\tau}{m_0} \cdot \begin{pmatrix} 6.364 \\ 1.4142 \\ -0.7071 \end{pmatrix},$$ project it into (110) direction:

$$j_{110} = \frac{ne^2\tau}{m_0} \cdot \frac{1}{\sqrt{2}}(1\,1\,0) \begin{pmatrix} 6.364 \\ 1.4142 \\ -0.7071 \end{pmatrix} \Rightarrow 5.5 \cdot \left(\frac{ne^2\tau}{m_0}\right).$$

$$\Rightarrow \sigma_{electron} = \overbrace{4 \times \sigma_{110}}^{\text{group A}} + 2 \times \overbrace{(4 \times \sigma_{011})}^{\text{group B or C}} = 48 \cdot \left(\frac{ne^2\tau}{m_0}\right);$$

$\therefore \sigma_h/\sigma_e \sim 0.3312$; Expected because electrons contribute more than holes due to their higher carrier mobilities.

h. Assuming $B = B\hat{z}$;

The standard way to solve the problem is to find out σ_B by taking into account of all contributions from electron pockets and hole pockets. Then,

$\vec{j} = \overleftrightarrow{\sigma_B} \cdot \vec{E}$; set $j_y = 0$, we can get E_y as a function of E_x; substitute into j_x expression, we can find out $\sigma_{xx}(B)$; and transverse magnetoresistance $\frac{\Delta\rho_{xx}}{\rho} = -\frac{\Delta\sigma}{\sigma} = -\frac{\sigma_{B_{xx}}(B) - \sigma_{B_{xx}}(0)}{\sigma_{B_{xx}}(0)}$;

In our case, this will be lots of algebra involved. Instead, we will estimate the contributions from various carrier types in an intuitive way. In general, transverse magnetoresistance is proportional to carrier mobility and density.

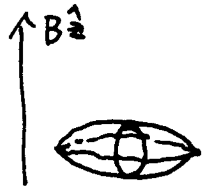
Let's consider electrons first:

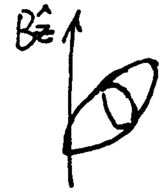
All electron pockets have the same carrier density, n, so it only depends on mobility, $\propto \omega_c\tau$, or, $\propto \frac{1}{m_c^*}$; $\left(\mu = \omega_c\tau \cdot \frac{c}{B}\right)$

For group A in (g), $m_c^* = \left(\frac{\det \overleftrightarrow{m^*}}{\hat{b}\cdot\overleftrightarrow{m^*}\cdot\hat{b}}\right)^{\frac{1}{2}} = 0.5771\, m_0$;

and for group B and C, for our field orientation, B and C will have same $m_c^* = \left(\frac{\det \overleftrightarrow{m^*}}{\hat{b}\cdot\overleftrightarrow{m^*}\cdot\hat{b}}\right)^{\frac{1}{2}} = 0.2356\, m_0$;

We can see that the results above are expected by looking at the following figures:





group A pockets have larger cross section $\perp$ B field and only $\frac{1}{3} m_0$ and m_0 component contribute $\Rightarrow$ larger cyclotron mass;

group B and C pockets have smaller cross section $\perp$ B field and m_0 component contributes less compare to group A $\Rightarrow$ smaller cyclotron mass;

Therefore, 8 electron pockets from group B and C contribute more to the magnetoresistance than group A pockets, because of their smaller $\omega_c \tau$;

Let's now look at the holes:

both heavy and light holes are spherical pockets, $\therefore m_c^* = m^*$;

But ~~remember~~ $n_i \propto m_i^{3/2}$, $\therefore \frac{n_i}{m_i} \propto m_i^{1/2}$, $\Rightarrow$

heavy holes dominate over light holes;

Now compare heavy holes and group B, C electrons,

$$\frac{n_{hh}}{m_{hh}} = \underbrace{\frac{12}{1+\frac{1}{3\sqrt{3}}}\cdot\frac{n}{m_0}}_{hh}, \quad \underbrace{\frac{8n}{0.2356\, m_0}}_{\text{B and C electrons}} = 34.0\ n/m_0,$$

$$= 10.1\ n/m_0,$$

$\Rightarrow$ electron pockets in group B and C contribute most to magnetoresistance.

2. 2 atoms p.u.c. per unit cell   L pts ($m_l^* = 0.3\,m_0$, $m_t^* = 0.1\,m_0$) - electron pockets

Γ pt ($m_h^* = 0.3\,m_0$) single hole pocket

L equivalent (111) directions   8 x ½ ellipsoids = 4 full electron pockets

a) $$n_{tot}^{electrons} = 4n_e = 4\int_0^\infty \left[\frac{1}{2\pi^2}\left(\frac{2}{\hbar^2}\right)^{3/2}\sqrt{m_{xx}m_{yy}m_{zz}}\right] E^{1/2} \frac{1}{e^{(E-E_F^e)/kT}+1}\, dE$$

pts. $$n_{tot}^{holes} = n_h = \int_0^\infty \left[\frac{1}{2\pi^2}\left(\frac{2}{\hbar^2}\right)^{3/2}\sqrt{m_{xx}m_{yy}m_{zz}}\right] E^{1/2} \frac{1}{e^{(E-E_F^h)/kT}+1}\, dE$$

Semimetal, so $n_{tot}^{electrons} = n_{tot}^{holes}$

Also $T=0$ so $f(E)$ is step function

$$n_{tot}^{electrons} = 4\int_0^{E_F^e} \frac{1}{2\pi^2}\left(\frac{2\pi}{\hbar^2}\right)^{3/2}\sqrt{m_l^* m_t^{*2}}\, E^{1/2} dE = \frac{2}{\pi^2}\left(\frac{2\pi}{\hbar^2}\right)^{3/2}\sqrt{m_l^* m_t^{*2}} \cdot \frac{2}{3}\cdot\left(E_F^e\right)^{3/2}$$

$$n_{tot}^{holes} = \int_0^{E_F^h} \frac{1}{2\pi^2}\left(\frac{2\pi}{\hbar^2}\right)^{3/2} m_h^{*\,3/2}\, E^{1/2} dE = \frac{1}{2\pi^2}\left(\frac{2\pi}{\hbar^2}\right)^{3/2} m_h^{*\,3/2} \cdot \frac{2}{3}\left(E_F^h\right)^{3/2}$$

Equating results of integrals

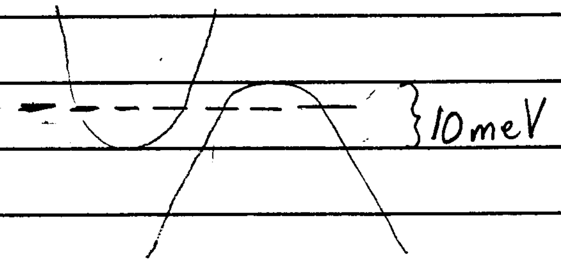
$$n_{tot}^{holes} = n_{tot}^{electrons} \Rightarrow 4\sqrt{m_l^* m_t^{*2}}\left(E_F^e\right)^{3/2} = m_h^{*\,3/2}\left(E_F^h\right)^{3/2}$$

Since $m_l^* = 0.3\,m_0$, $m_t^* = 0.1\,m_0$ & $m_h^* = 0.3\,m_0$

$$\therefore E_F^e = \frac{0.3}{(0.219)^{2/3}} E_F^h$$

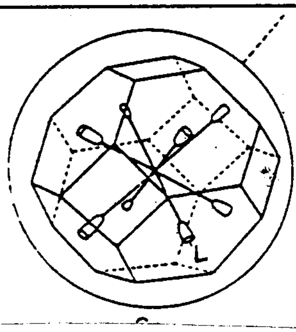
$$E_F^e = 0.83\, E_F^h$$

Also $E_f^e + E_f^h = 10\,meV$



$\therefore \quad E_f^h = 5.5\,meV$

$E_f^e = 4.5\,meV$



Interpocket scattering between electron pockets

Scattering between L pts, smallest $\vec{q}$ such as from

from $(11\bar{1})$ to (111) pocket

$\vec{k}' = (1,1,1)\left(\frac{\pi}{a}\right)$

$\vec{k} = (1,1,\bar{1})\left(\frac{\pi}{a}\right)$

$\vec{k}' = \vec{k} + \vec{q}$

$\vec{q} = \vec{k}' - \vec{k} = (0,0,2)\left(\frac{\pi}{a}\right)$ which is half of a reciprocal lattice vector.

$|\vec{q}| = \frac{2\pi}{a}$

If unklapp processes were to occur

$\vec{k}' = \vec{k} + \vec{q} + \vec{G}$ where $\vec{G}$ is a reciprocal lattice vector.

The shortest $\vec{G}$'s for the fcc lattice are the eight vectors $(2\pi/a)(\pm1, \pm1, \pm1)$.

It would take an electron say from the (111) pocket to the $(\bar{1}\bar{1}1)$ pocket

$$\vec{k}' - \vec{k} = \frac{\pi}{a}\left\{(\bar{1}\bar{1}1) - (111)\right\} = (\bar{2}, \bar{2}, 0)\left(\frac{\pi}{a}\right)$$

$$\therefore \vec{q} + \vec{G} = (\bar{2}, \bar{2}, 0)\left(\frac{\pi}{a}\right)$$

If we use the reciprocal lattice vector $\vec{G} = \left(\frac{2\pi}{a}\right)(\bar{1}, \bar{1}, \bar{1})$

$$\vec{q} = \left(\frac{\pi}{a}\right)\left[(\bar{2}, \bar{2}, 0) - (\bar{2}, \bar{2}, \bar{2})\right]$$

$\vec{q} = \left(\frac{\pi}{a}\right)(0, 0, 2)$ which is the wavevector found in part (b).

d) Quantum well with (001) crystalline direction normal to thin layer of semimetal. $L = 50\,\mathring{A}$

The energies are quantized in the $\hat{z}$ direction

$$E = \frac{\hbar^2}{2}\left[\frac{k_x^2}{m_{xx}} + \frac{k_y^2}{m_{yy}}\right] + \frac{\hbar^2}{2m_{zz}}\left(\frac{n\pi}{L}\right)^2$$

For the $(1,\bar{1},\bar{1})$ pocket

$$\left(\overleftrightarrow{\frac{1}{m^*}}\right)_{crystal} = \begin{pmatrix} \frac{1}{m_\ell} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_t} \end{pmatrix}$$

$$\left(\overleftrightarrow{\frac{1}{m^*}}\right)_{lab} = R\left(\overleftrightarrow{\frac{1}{m^*}}\right)_{crystal} R^{-1}$$ where R rotates vectors from crystal coord. to lab coordinates.

From Problem Set # 3

$$R_{(1\bar{1}\bar{1})} = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} & 0 \\ -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \end{pmatrix} \qquad R^{-1}_{(111)} = \begin{pmatrix} \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

Result is: $$\left(\overleftrightarrow{\frac{1}{m^*}}\right)_{lab} = \begin{pmatrix} \frac{1}{3m_\ell} + \frac{2}{3m_t} & -\frac{1}{3m_\ell} + \frac{1}{3m_t} & -\frac{1}{3m_\ell} + \frac{1}{3m_t} \\ -\frac{1}{3m_\ell} + \frac{1}{3m_t} & \frac{1}{3m_\ell} + \frac{2}{3m_t} & \frac{1}{3m_\ell} - \frac{1}{3m_t} \\ -\frac{1}{3m_\ell} + \frac{1}{3m_t} & \frac{1}{3m_\ell} - \frac{1}{3m_t} & \frac{1}{3m_\ell} + \frac{2}{3m_t} \end{pmatrix}$$

$\therefore \frac{1}{m_{zz}} = \frac{1}{3m_l} + \frac{2}{3m_t}$

* This could have also been found by finding the longitudinal effective mass

$$\frac{1}{m_l^*} = \hat{b} \cdot \left(\overleftrightarrow{\frac{1}{m^*}}\right) \cdot \hat{b}$$

$$\left(\frac{1}{m_l^*}\right) = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right) \begin{pmatrix} \frac{1}{m_l} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_t} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}$$

$$\frac{1}{m_{z}} = \frac{1}{3m_l} + \frac{2}{3m_t}$$

$\therefore$ The energy of the lowest L subband

(Set $n=1$) $\quad E = \frac{\hbar^2}{6m_0}\left(\frac{1}{0.3} + \frac{2}{0.1}\right)\left(\frac{\pi}{L}\right)^2 = \frac{\hbar^2}{6m_0}(23.3)\left(\frac{\pi}{L}\right)^2$

$$E = 3.88 \frac{\hbar^2}{m_0}\left(\frac{\pi}{L}\right)^2$$

e) Transition occurs when the lowest subband of the electrons and holes just cross.

$$\Delta E_{elec} + \Delta E_{holes} = 10\,meV$$

$$\left[\frac{\hbar^2}{6m_o}(23.3) + \frac{\hbar^2}{2m_o}(3.33)\right]\left(\frac{\pi}{L}\right)^2 = 10\,meV$$

$$L^2 = 4.18 \times 10^{-16}\,m^2$$

$$L \approx 20\,\text{Å}$$

f) If grown along a (111) direction, then the hole contribution remains the same. One full electron pocket is along the (111) direction and has the largest effective mass $\left(\frac{1}{m^*} = \frac{1}{m_\ell}\right)$. The other three electron pockets contribute smaller effective masses because they are tilted w.r.t. the (111) direction and their terms involve mixing of the light & heavy mass components. The light mass subband moves up faster with the narrowing of the well. The semimetal to semiconductor transition therefore depends on the motion of the heavy mass subband for the electrons.

$$\frac{\hbar^2}{2m_0}\left[\frac{1}{0.3}+\frac{1}{0.3}\right]\left(\frac{\pi}{L}\right)^2 = 10\,meV$$

$$L^2 = 2.5\times10^{-16}\ m^2$$

$$L = 16\,\mathring{A}$$

The well width must be narrower for the transition to occur.

g) At low temperature all carriers are in their lowest energy state. Low temperature optical experiments could then be performed to monitor the onset of transition. Since the material is indirect gap, this will be difficult.

A low temperature transport measurement, such as a Hall measurement, would also indicate the onset of the semimetal - semiconductor transition.