Simulation of critical temperature of FeTe, FeSe and FeTe$_{0.5}$Se$_{0.5}$ using equation McMillan

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Abstract. This study uses simulation to produce the critical temperature of FeTe, FeSe, and FeTe$_{0.5}$Se$_{0.5}$ superconductors using McMillan equation which show shifts in $\lambda$ (electron-phonon coupling strength), $\bar{\omega}_{\text{ph}}$ (logarithmic average of phonon frequency), and Density of States (DOS) at the Fermi level compared to its composing elements. Comparison of critical temperatures shows that Fe mixed with Se and/or Te experience some changes that could possibly increase of the critical temperature.

Keywords: Critical temperature, McMillan equation, simulation

1. Introduction
Since the discovery of superconductivity on FeSe [1], many studies have been conducted in order to understand the superconductivity of Fe-chalcogenides. Fe-chalcogenides have several types of crystal structures such as the anti-PbO-type and the NiAs-type. The common compounds of Fe-chalcogenides that have been mostly observed is the one with the anti-PbO-type crystal structures. Several compounds of Fe-chalcogenides that have this type of crystal structure are FeS, FeSe and FeTe [2]. In this phase, FeSe exhibits superconductivity while FeTe does not show any superconductivity [3]. However, if Se is doped into the material, FeTe$_{1-x}$Se$_x$ shows superconductivity. Thus, in this study we aim to calculate the critical temperature of FeSe, FeTe, FeTe$_{0.5}$Se$_{0.5}$ and its constituent element (Fe, Te, and Se). Furthermore, we also want to take into account: changes of electron-phonon coupling strength, logarithmic average of phonon frequency, and the density of states to the magnitude of the critical temperature. Here, we use simulation then the apply the McMillan equation to obtain the critical temperature of each material.

2. Method
McMillan equation is based on the Eliashberg theory [4] which is an extension from BCS theory [5]. The main point of Eliashberg theory is the Coulomb repulsion which is defined as,

$$\mu = N(0)|\zeta|$$  \hspace{1cm} (1)$$

where $\mu$ is the instantaneous Coulomb repulsion, $N(0)$ is the density of single spin from the electronic
state at the Fermi level and $|V_c|$ is the potential. Besides the Coulomb repulsion, another main point of Eliashberg theory is the spectral function of electron phonon which defined as,

$$
\alpha^2F(\omega) = N(0)\sum_{kk'}|M_{kk'}|^2 \delta(\omega - \omega_{Q})\delta(\epsilon_k)\delta(\epsilon_{k'})
$$

(2)

where $\alpha^2F(\omega)$ is the spectral function of electron-phonon, $Q = k - k'$ with $Q$ and $k$ being the wave number and the band quantum number for phonon and electron, $\omega_Q$ and $\epsilon_k$ is the energy of phonon and electron respectively and $M_{kk'}$ is the matrix element of electron-phonon coupling.

McMillan then found a solution of Eliashberg theory for finite temperature to determine the critical temperature, $T_c$, for any cases. McMillan defined the critical temperature, $T_c$, as,

$$
T_c = \frac{\theta_D}{1.45} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)
$$

(3)

Here, $\theta_D$ is the Debye temperature, $\lambda$ is the strength of electron-phonon spectral function $\alpha^2F(\omega)$ and $\mu^*$ is the effective Coulomb repulsion. However, Dynes [6] then introduced further changes to equation 3 where $\frac{\theta_D}{1.45}$ is corrected to $\frac{\langle\omega\rangle}{1.20}$ with $\langle\omega\rangle$ is the average phonon energy. Thus, equation 3 is then transformed into,

$$
T_c = \frac{\langle\omega\rangle}{1.20} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right).
$$

(4)

Then, using McMillan equation, the critical temperature can be calculated as,

$$
T_c = \frac{\omega_{log}}{1.2} e^{-\frac{1.04(1+\lambda)}{\lambda(1-0.62\mu^*)-\mu^*}}.
$$

(5)

where

$$
\mu^* = \frac{V_c N(0)}{1 + V_c N(0)\ln \left(\frac{E_F}{\omega_p}\right)}
$$

(6)

and

$$
\omega_{log} = e^{\frac{\alpha^2 F(\omega)}{\omega}} \frac{d\omega}{d\alpha^2 F(\omega) log(\omega)}.
$$

(7)

We then perform the simulation of Fe, Te, Se, FeTe, FeSe and FeTe$_{0.5}$Se$_{0.5}$. Using Quantum Espresso 6.0 in the simulation, we obtain several variables such as density of states, Fermi energy, $\omega_{log}$, $\lambda$ and the ratio between $\lambda$ and $T_c$. Then, the critical temperature for each material is calculated using equation 5 to equation 7.
3. Results and discussion

Using Quantum Espresso, we have simulated the Fe, Te, Se, FeSe, FeTe, and FeTe0.5Se0.5 and have obtained the critical temperature ($T_c$), $\lambda$, $\omega_{\log}$, density of states at the Fermi level (DOS ($E_F$)) and the energy Fermi as shown in table 1. Our simulation of Fe shows that Fe has $T_c$ of 0.01 K and a BCC structure. Our results are different with the previous study [7]. The study have shown that Fe at ambient pressure which has a BCC structure do not exhibit superconductivity phenomenon. We also obtain that at the Fermi level the density of states of Fe is 2.43 eV$^{-1}$m$^{-3}$ while the $\lambda$ is 1.20. So, the difference between these values for Fe is relatively small. The value of $\omega_{\log}$ which equals to 25.93 THz is small, thus, it does not give a significant contribution in enhancing the value of the critical temperature of Fe.

The simulations of Te and Se shows that the critical values are 0.64 K and 2.23 K, respectively, and both have the hexagonal crystal structure. Similar to Fe, the results are different with previous study [7] which shows that Te and Se are not superconductor at normal pressure. The values of $\omega_{\log}$ for both elements is quite large, that is, 73.61 THz and 62.18 THz, respectively. However, the large value of $\omega_{\log}$ of those elements does not correspond to a large value of critical temperature, $T_c$. This is due to the small value of $\lambda$ of both elements in which 0.19 for Te and 0.27 for Se.

For FeTe, we found that the critical temperature, $T_c$, of FeTe is 0.006 K and the crystal structure of FeTe is tetragonal. Our simulation which shows that FeTe has a critical temperature is different with previous study [8] which shows that FeTe is not a superconductor. FeTe has DOS at the Fermi level at 20.17 eV$^{-1}$m$^{-3}$ with $\lambda = 0.11$ and $\omega_{\log} = 83.23$ THz. Compare to its constituent element, Fe and Te, $\lambda$ is smaller. $\lambda$ of Fe is greater than 1 which means that Fe has a strong coupling while $\lambda$ value of Te which smaller than 1 correspond to the weak coupling for Te. When Fe and Te are combined, the $\lambda$ values drop dramatically to the area of weak coupling ($\lambda < 1$). At Fermi Level, the density of states of FeTe is greater than Te but smaller than Fe. The Fermi energy of FeTe decrease so its value is smaller than the Fermi energy of Fe, although it is still greater than the Fermi energy of Te. We could see that there is a slight enhancement on the $\omega_{\log}$ value of FeTe compared to its constituent elements however the small value of $\lambda$ induce the small value of $T_c$.

Previous study of FeSe has observed that the $T_c$ of this material is about 8–13 K [9, 10] in agreement with our results. Our simulations shows that the $T_c$ of FeSe is 12.4 K with tetragonal structure which also in agreement with the literature [9]. The critical temperature of FeSe excess its constituent elements. The DOS of FeSe at the Fermi level and its value of $\omega_{\log}$ is greater than Fe and Se, differ from FeTe where both values are smaller than Fe. The value of $\lambda$ of FeSe do not decrease dramatically although the value is still smaller than Fe. However, the $\lambda$ value of FeSe is greater than Se as one of its constituent element. For FeSe, $\lambda = 1.19$ which greater than 1 correspond to a strong coupling that occur in this material. The values of $\lambda$, $\omega_{\log}$, and DOS at Fermi level of FeSe contribute to a critical temperature that far exceeds the critical temperature of its constituent elements.

For FeTe0.5Se0.5, the simulation obtain a hexagonal crystal structure and $T_c = 12.2$ K which is smaller than the experimental result [11]. The magnitude of the critical temperature of this material is greater than its constituent element but almost the same as critical temperature of FeSe. The value of Fermi energy of FeTe0.5Se0.5 is smaller than FeSe but greater than FeTe. Meanwhile its $\lambda$ is greater than the value of $\lambda$ of its constituent elements and FeTe also FeSe. This value pass over the limit of

| Table 1. Simulation results |
|-----------------------------|
| $T_c$ (K) | $\lambda$ | $\omega_{\log}$ | DOS($E_F$) (eV$^{-1}$m$^{-3}$) | $E_F$ (eV) |
| Fe | 0.01 | 1.2 | 25.93 | 2.43 | 16.81 |
| Te | 1.77 | 0.38 | 73.62 | 10.5 | 1.92 |
| Se | 2.23 | 0.27 | 62.18 | 7.02 | 5.17 |
| FeTe | 0.06 | 0.11 | 83.23 | 20.17 | 9.34 |
| FeSe | 12.4 | 1.19 | 105.15 | 16.65 | 16.34 |
| FeTe0.5Se0.5 | 12.2 | 1.49 | 89.13 | 16.49 | 15.97 |
the weak coupling, so it has a strong interaction coupling. The density of states at the Fermi level for FeTe$_{0.8}$Se$_{0.2}$ is greater than those of its constituent elements and close to the value of FeSe while the value of $\omega$log is greater than its constituent elements and FeTe but is smaller than FeSe. Our results shows that a partial substitution of Te with Se contributes to the $\lambda$, $\omega$log and DOS at the Fermi level so that the critical temperature of FeTe$_{0.8}$Se$_{0.2}$ exceed the critical temperature of FeTe and slightly smaller than the critical temperature FeSe.

4. Conclusion
We have simulated the Fe, Te, Se, FeTe, FeSe, and FeTe$_{0.5}$Se$_{0.5}$ using quantum espresso. From the discussion, it can be concluded that the critical temperature of FeSe and FeTe$_{0.5}$Se$_{0.5}$ has far exceeded its constituent elements. FeTe has lower $T_c$ than its constituent elements. The simulation results show the value of $T_c$ of FeSe, and FeTe$_{0.5}$Se$_{0.5}$ correspond to the experimental results.

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