Returnable Electron-Phonon Interaction in the II-VI Compound Alloys

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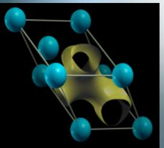
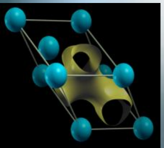


The phonon spectra

of $Hg_{1-x}Cd_{x}Te$ (MCT)

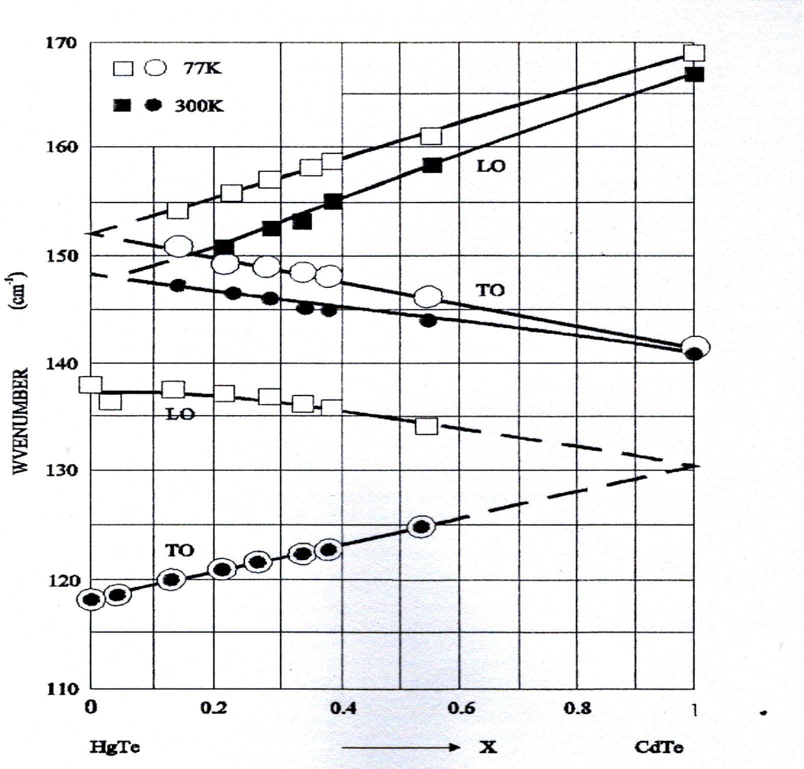
Mismatch of lattices is less than 0.1 %

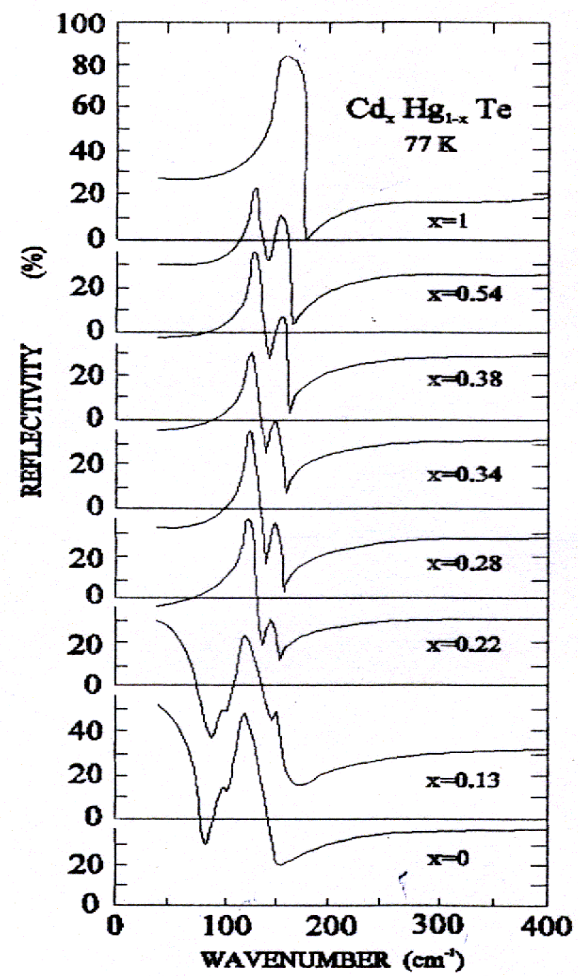
Zero Gap State – singularity in the band–structure

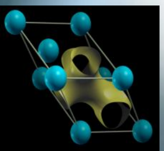


The phonon spectra of $Hg_{1-x}Cd_xTe$ (MCT)

J.Baars and F.Sorgers, *Solid State Commun.*, **10,** 875(1972)



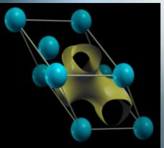




The phonon spectra of $Hg_{1-x}Cd_xTe$ (MCT)

1. D.N. Talwar , *J.Appl.Phys*. **56**, 1601 (1984).
2. 2. P.M. Amirtharaj, N.K. Dhart, J. Baars and H.Seelewind, *Semicond. Sci. Technol*. **5,** S68(1990).
3. S. Rath, K.P. Jain, S.C. Abbi, C. Julien, M. Balkanski, *Phys . Rev. B* ,**52,** 24, 17172 (1995).
4. Li. Biao ,J.H.Chu, H.J. Ye, S.P. Guo,W.Jiang, D.Y.Tang, *Appl.Phys.Lett*. **68,**23,3272,(1996).
5. 5. S.P.Kozyrev, L.K. Vodopyanov, R.Triboulet, *Phys. Rev.B*, **58**, 3, 1374 (1998).
6. Li. Biao, *Appl.Phys.Lett*, **73**, 1538 (1998).
7. J.Cebulski, E.M. Sheregii, J.Polit, A.Marchelli, M. Piccinini, A. Kisiel, I.V.Kucherecho, R. Triboulet, *Apll. Phys. Lett*. **92**, 121904 (2008).
8. E.M. Sheregii, J. Cebulski, A. Marcelli and M. Piccinini, *Phys. Rev. Lett*. **102,** 045504, (2009)

- **Additional lines in the 100 cm^{-1} -115 cm^{-1} region (All communications)**
- **Abnormal temperature dependence of the HgTe-like phonon mode frequency (**S. Rath, at al., *Phys . Rev. B* ,**52,** 24, 17172 (1995); E.M. Sheregii, at al., *Phys. Rev. Lett*. **102,** 045504, (2009))
- **Subtle structure of maine spectral subbands (All communications)**



Electron-Phonon Interaction

In the multi-mode medium each phonon mode produces his own polar potential

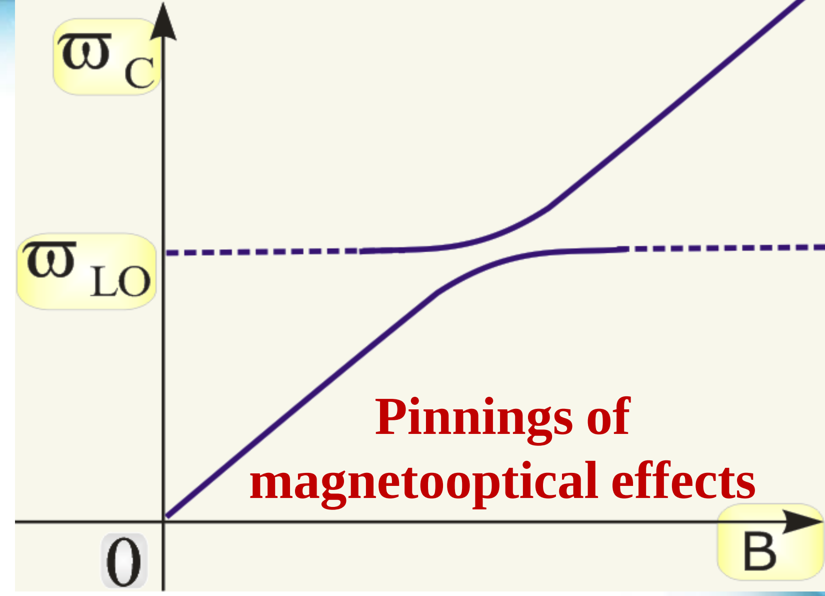
$$V_q^s = \frac{\hbar\omega_{LOs}}{qu^{1/2}}\left(\frac{4\pi\alpha_s}{V}\right)^{1/2}$$

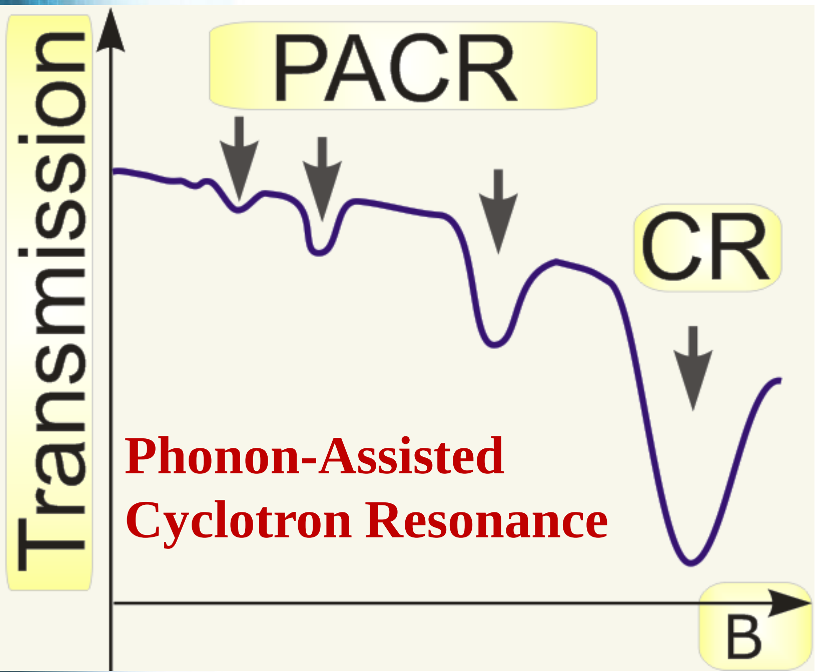
D. Płoch, E.M. Sheregii, M. Marchewka, M. Woźny and G. Tomaka, *Phys. Rev. B* **79**,195434 (2009)

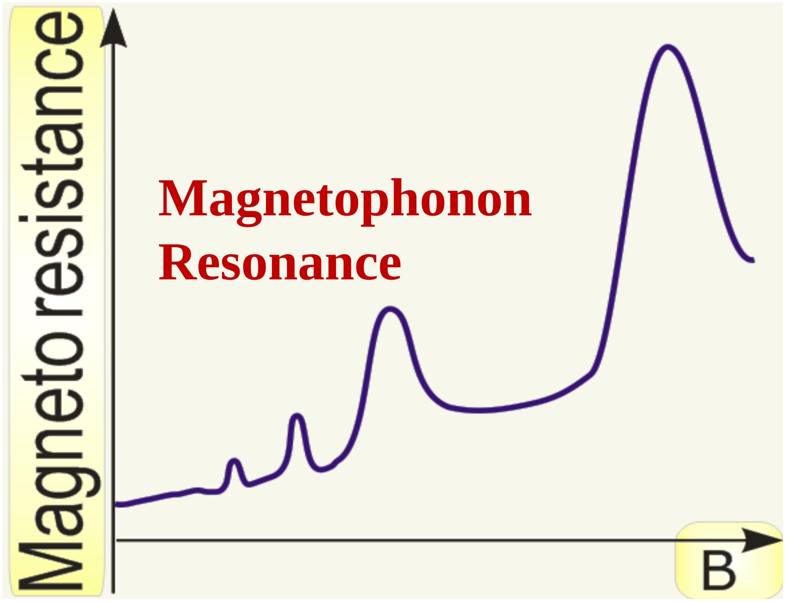
It is a direct electron-phonon interaction

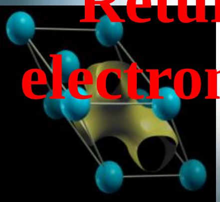
Direct Electron-Phonon Interaction

causes several resonances in semiconductors:



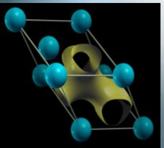






Returnable resonance electron-phonon interaction – electrons influence on the phonon spectrum – are known less

Zero Gap State – singularity in the band–structure

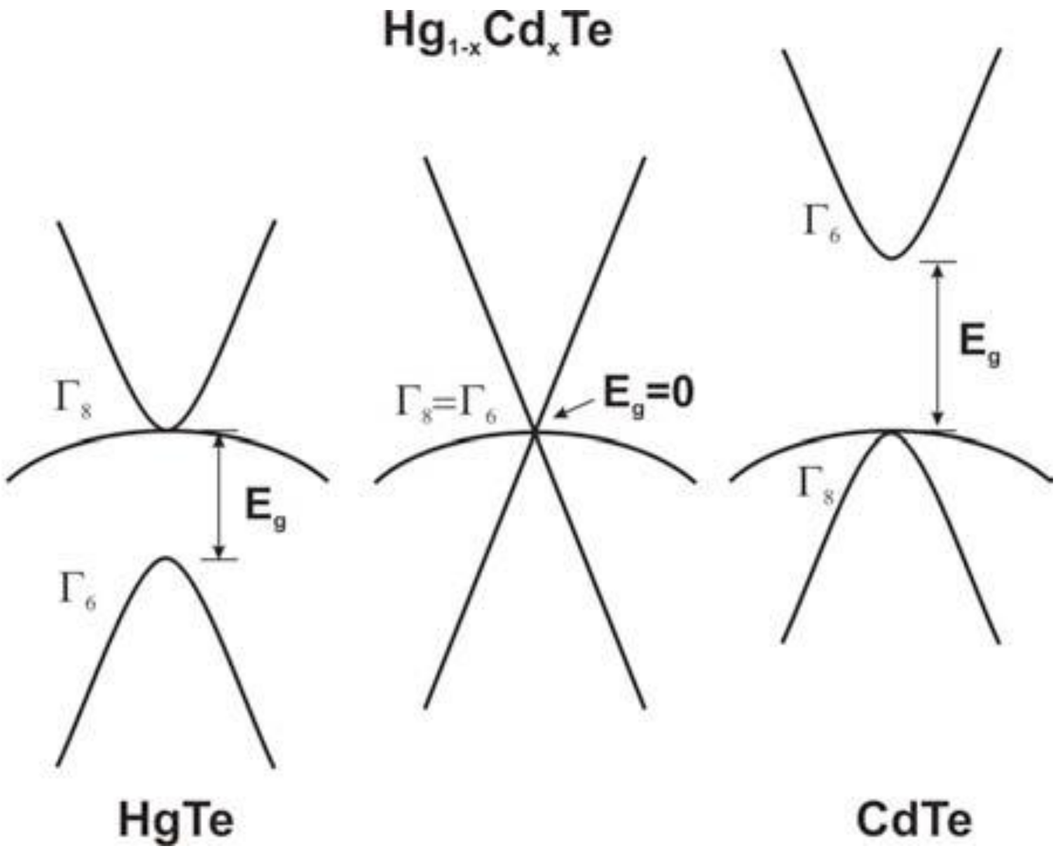


Zero Gap State – singularity in the band–structure

In the HgCdTe (MCT) alloys a zero-gap state

$$E_g \equiv \Gamma_6 - \Gamma_8 = 0$$

may occur as the composition varies from HgTe to CdTe.



This singular mechanism of the E_g variation may be triggered by an external pressure or by a temperature.

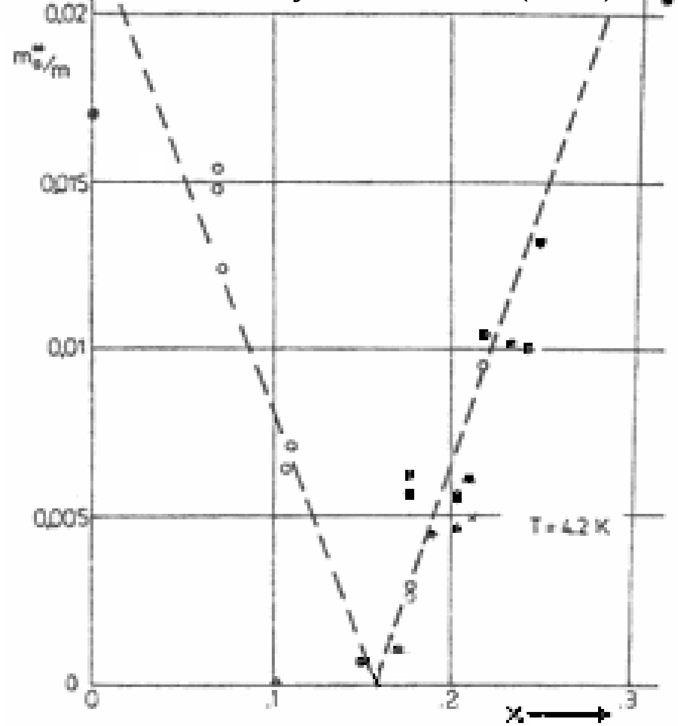
Singularity in the band structure

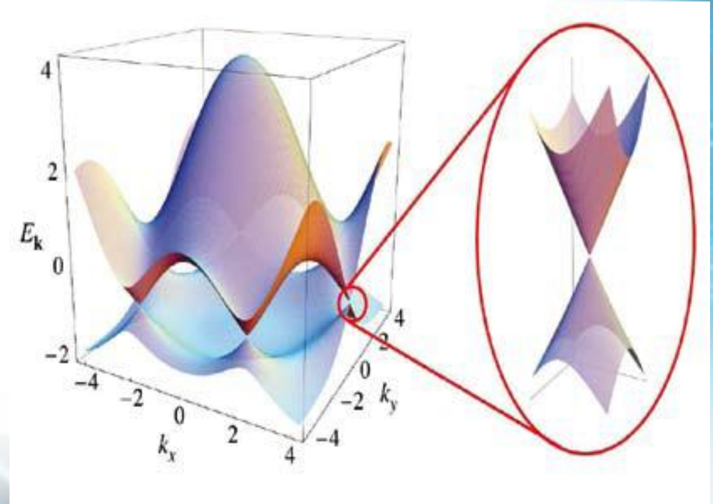
According to the Kane's theory [E. Kane, J. Phys. Chem. Solids **1**, 82 (1956).] for the compositions with a zero-band gap the electron effective mass at the conduction band edge should be equal to zero – experiment's data shown that it is really close to zero.

Many physical properties are then strongly affected by this singular characteristic of the band-structure of such alloys.

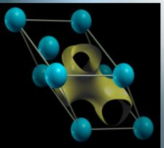
Now, this singularity is known as Dirac point existed in graphene

R. Dornhaus, G. Nimitz, *Sol. St. Phys.*, 78, 1-119, (1976).





Mechanism of the electron-phonon coupling



Mechanism of the electron-phonon coupling

It is necessary to identify

the electron-phonon interaction mechanism

to analyse the influence of

the zero-gap state

to

the phonon spectra

The transverse optical (*TO)* phonons

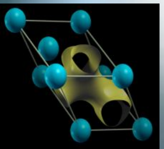
are only clearly recognized in

the optical reflectivity experiments

The preferred mechanism

for the interaction of electrons with TO-phonons is

a deformation potential



The electron-phonon coupling constant

for the *TO*-phonons with a small wave vector q, is:

$$V_{n,n'}(k,q,s) = \left(\frac{\hbar}{2MN\omega_{TO}}\right)^{\frac{1}{2}} \frac{1}{a} \Xi_{n,n'}(k,q) e(q,s)$$

the optical deformation potential matrix is:

$$\Xi_{n,n'}(k,q) = a \int \psi_{n',k+q} \frac{\partial V}{\partial u} \psi_{n,k} dr$$

the self energy of the *TO*-phonons with small wave-vector q is:

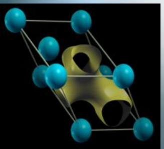
$$\omega_{TO}^{*2} = \omega_{TO}^{2} - \int dEF(E) \left\{ \frac{1}{E + E_g + \hbar\omega_{TO}} + \frac{1}{E + E_g - \hbar\omega_{TO}} \right\}$$

H. Kawamura, S. Katayama, S. Takano, S. Hotta, Solid State Comm. **14,** 259 (1974)

Two kinds of singularity could be predicted:

First one: $\hbar\omega_{TO} = E_g$

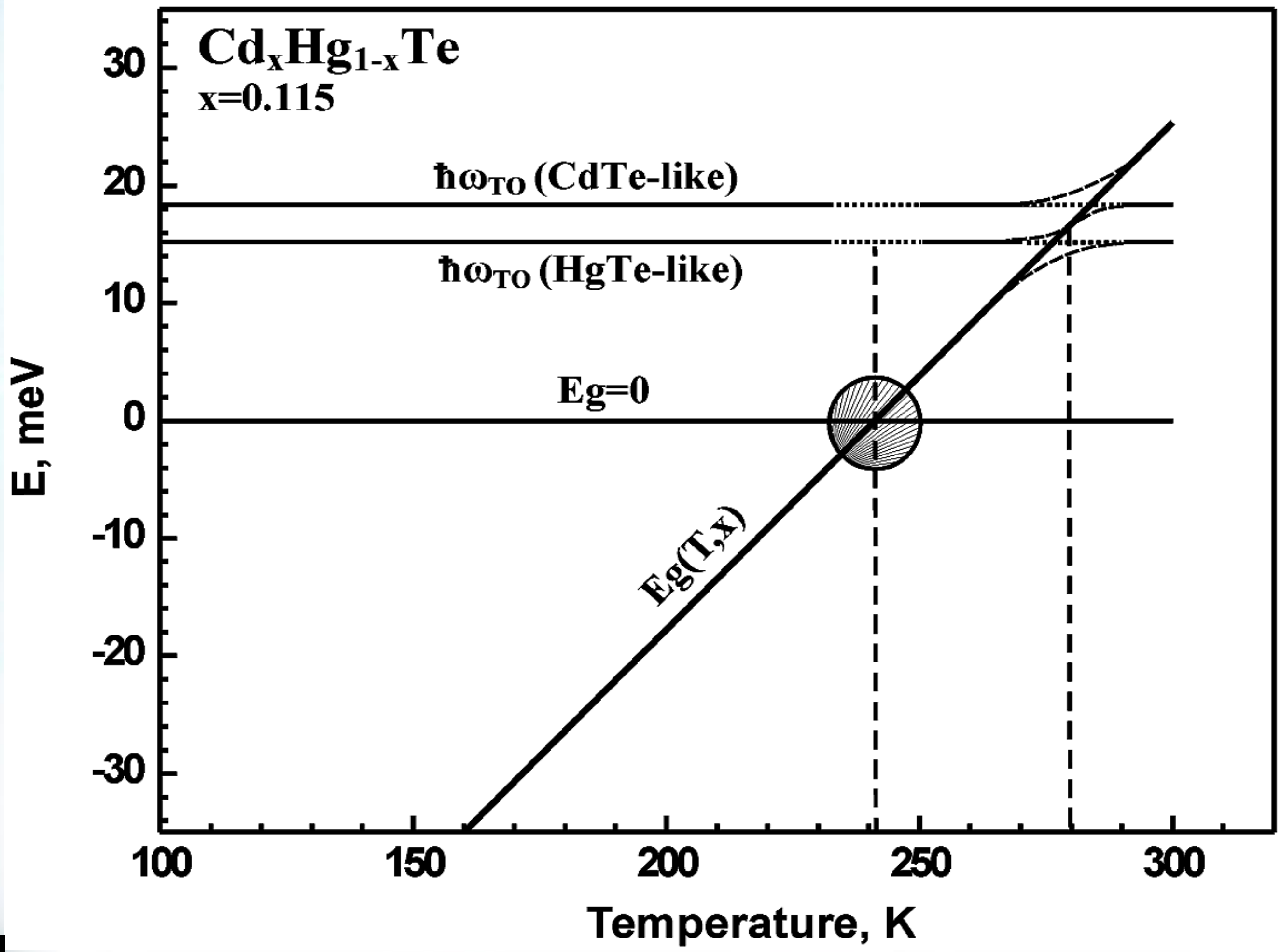
Second one: $E_g(T) = 0$



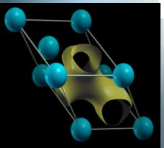
The singular mechanism of the E_g variation may be triggered by a temperature in the HgCdTe alloys

$$E_g(x,T) = -0.303 + 1.73x + 5.6\cdot 10^{-4}(1-2x)T + 0.25x^4$$

M. W. Scott, JAP, **40**, 4077 (1969)



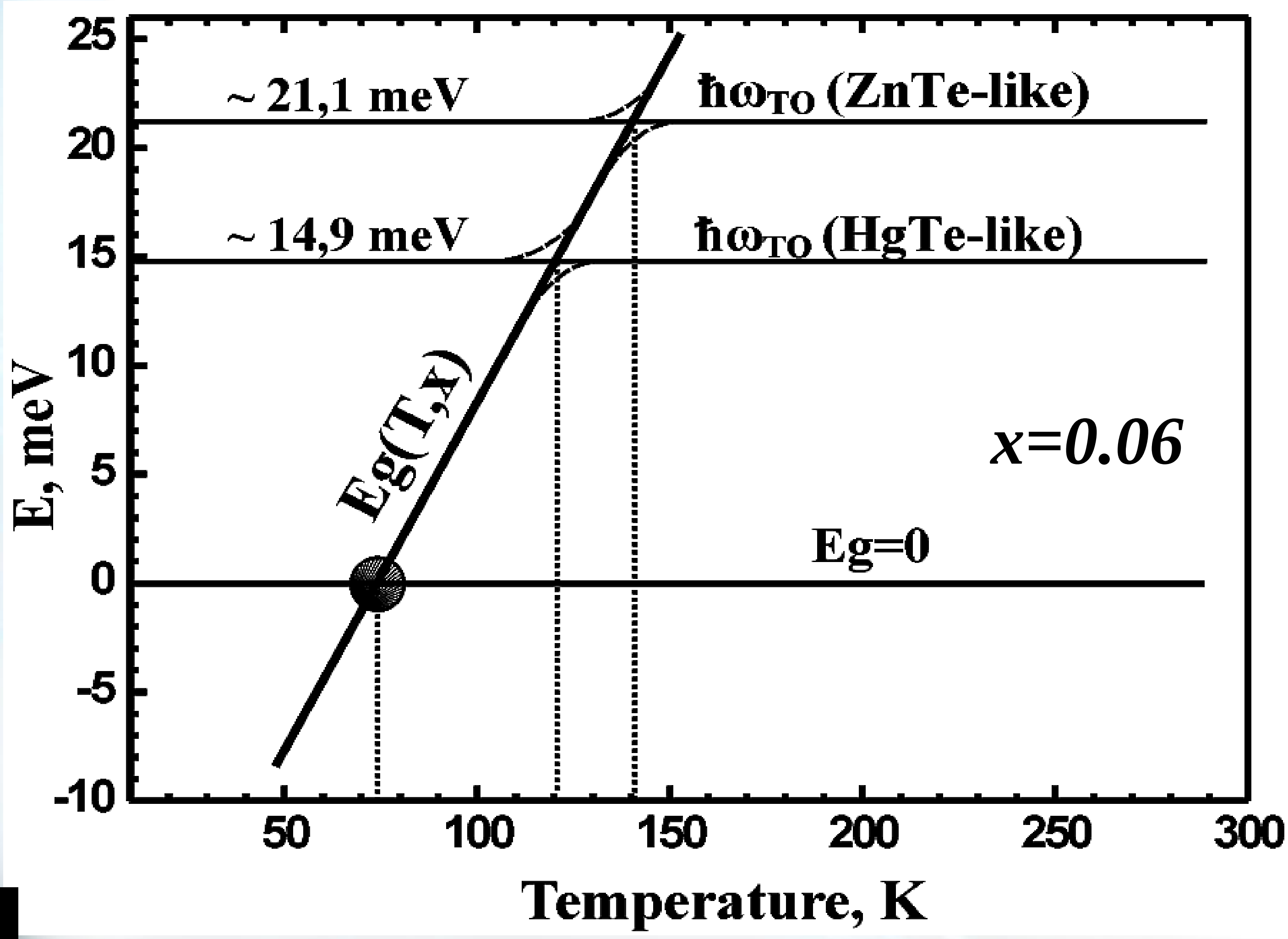
In the $Hg_{1-x}Cd_xTe$ (x = 0.115) alloy a zero-gap state $E_g \equiv \Gamma_6 - \Gamma_8 = 0$ takes place at approximately 242 K



Similar situation is in HgZnTe Alloys

Empirical formula $E_g(x,T)$ was derived for this alloys:

$$E_g(x,T) = -0.302 + 2.731x + 3.24\cdot 10^{-2} x^{1/2} - 0.629x^2 + 0.533x^3 + 5.3\cdot 10^{-4}(0.76x^{1/2} - 1.29x)T$$



A. Sher, at al. J. Vac. Sci. Techn. ***A 4*** *2024 (1986)*]

Singularity takes place at 83 K

EXPERIMENT

EXPERIMENT

A brilliant and intense

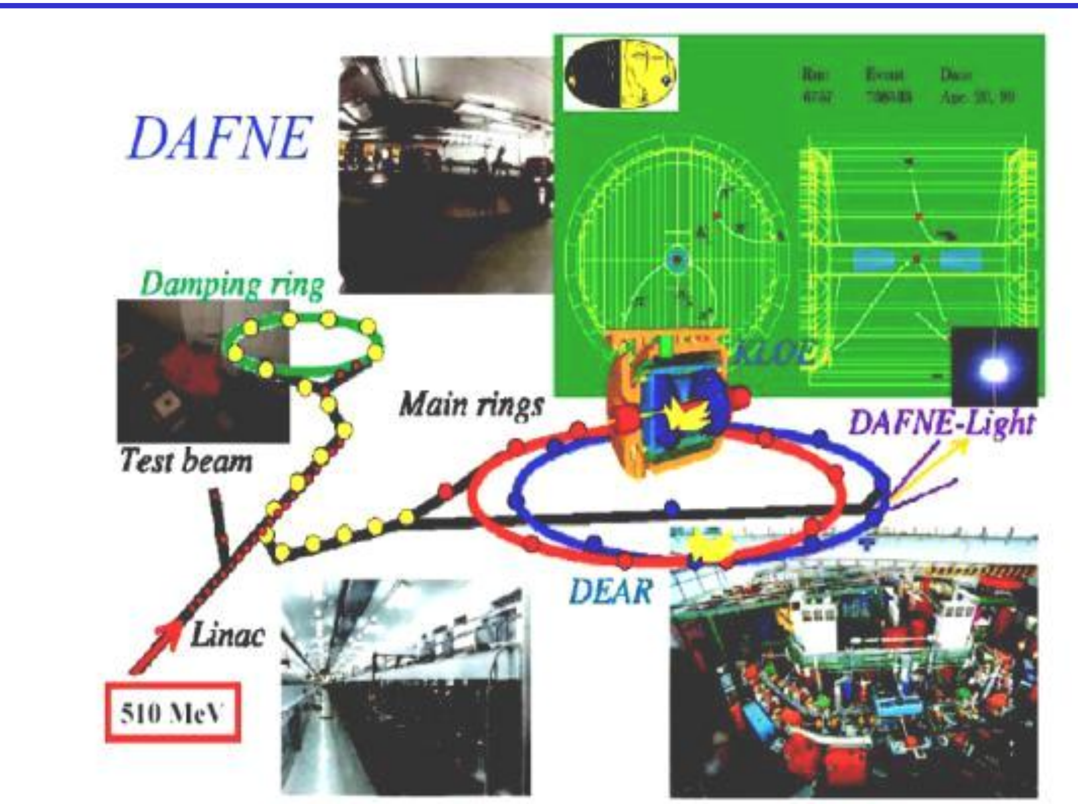
synchrotron radiation (SR)

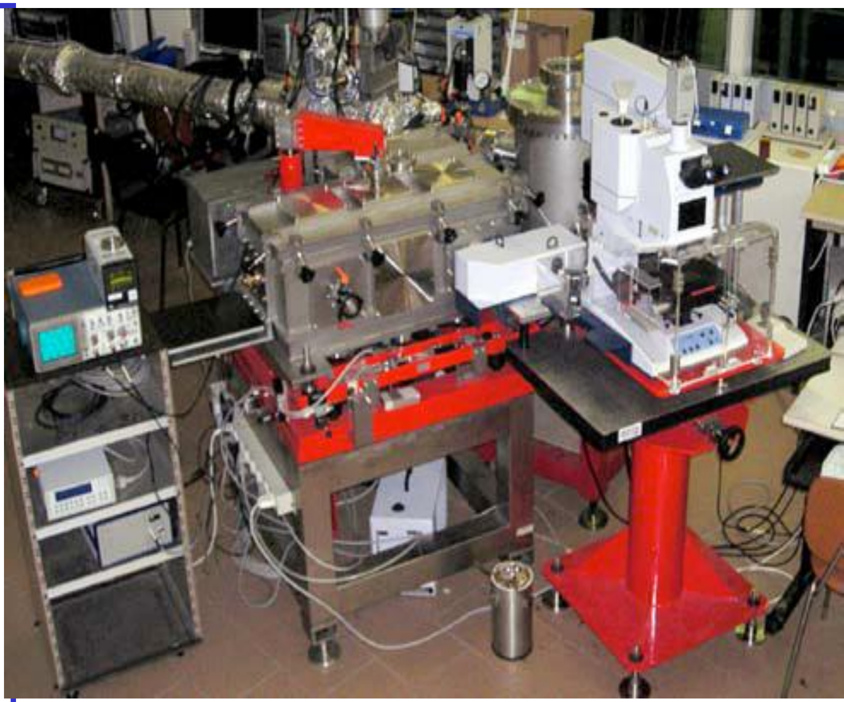
in the far infrared domain offers unique advantages

Far Infrared reflectivity experiments

were performed at

the DAFNE-light laboratory at Frascati (Italy)

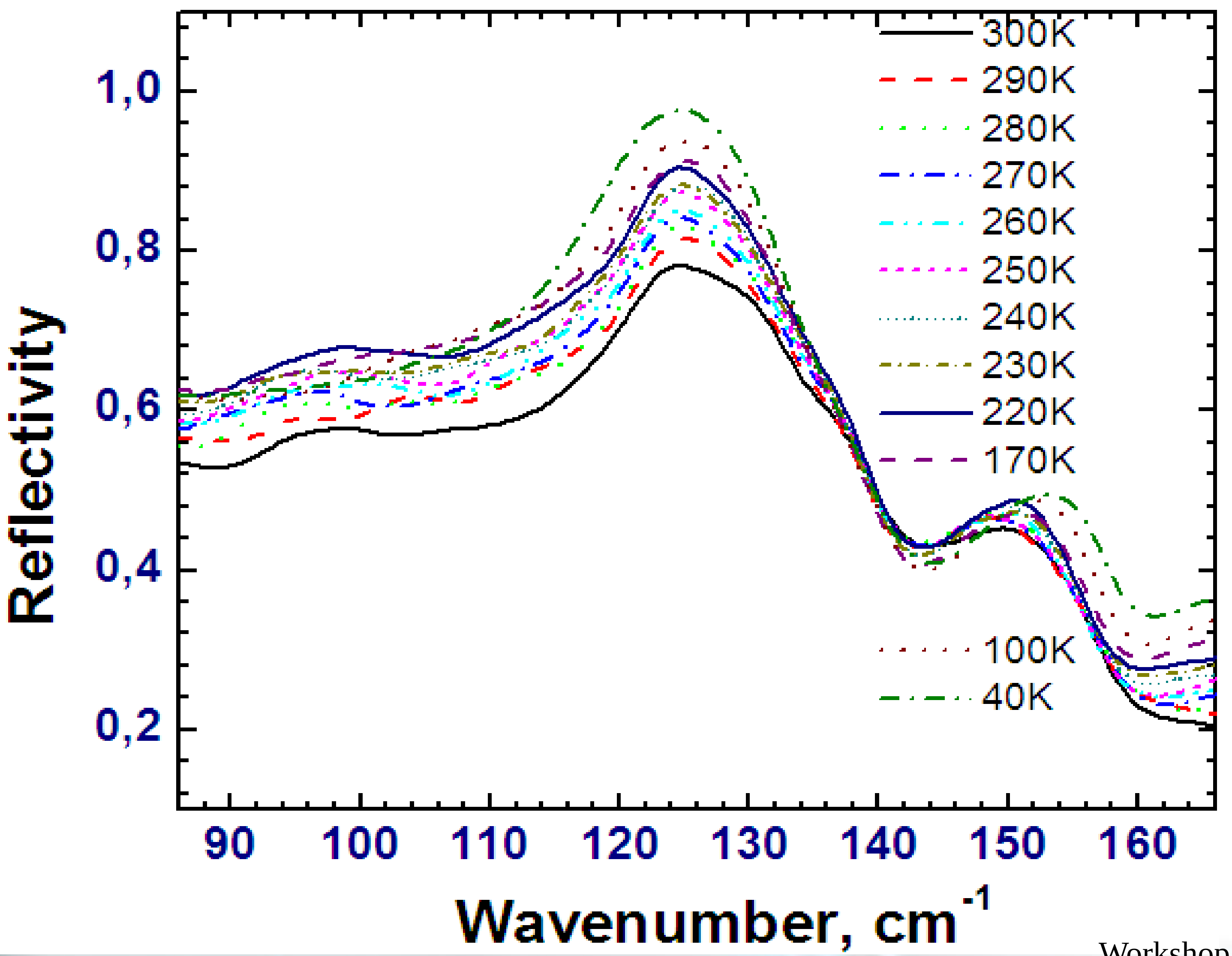




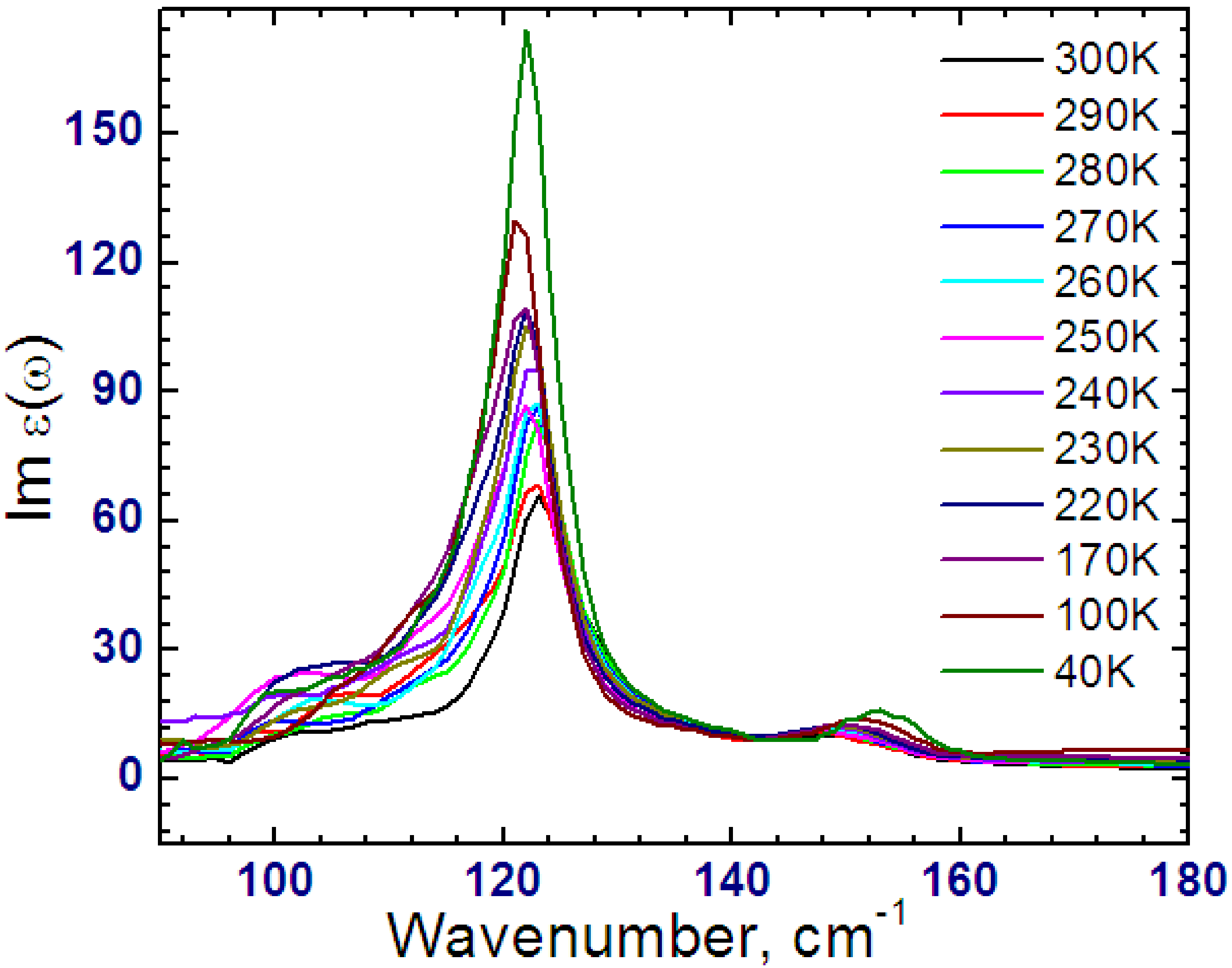
The optical reflectivity experiment

in the far-infrared region

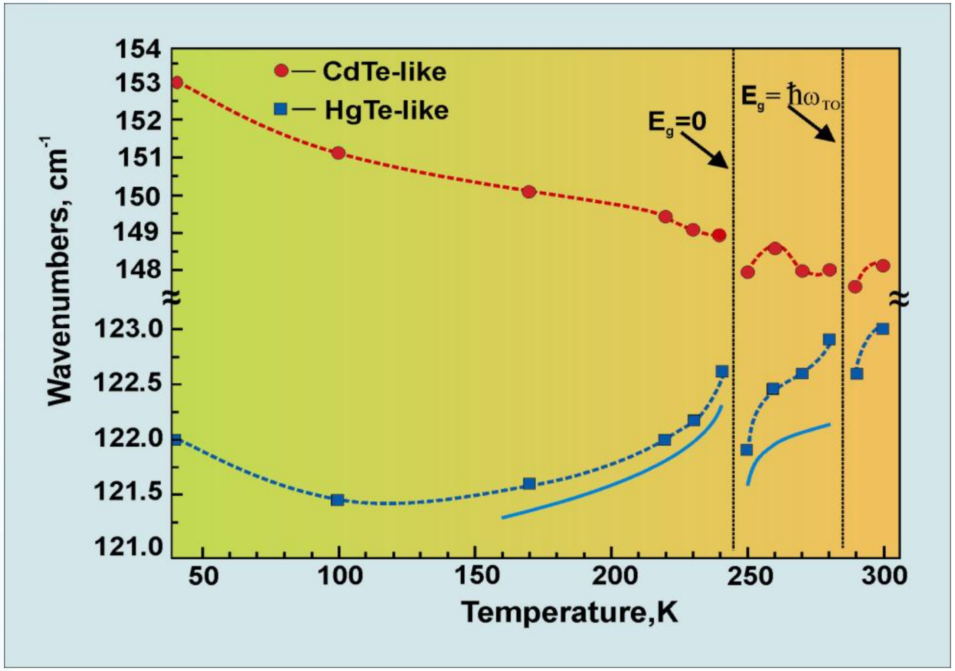
$Hg_{1-x}Cd_xTe$ (x=0.11)

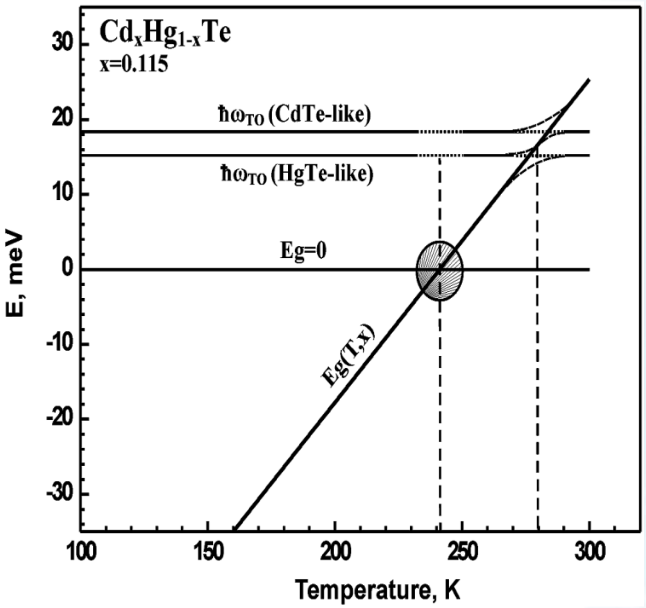


The dielectric function
Imaginary part
$Hg_{1-x}Cd_xTe$ (x=0.11)



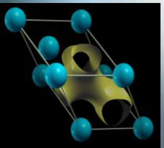
The frequency positions
vs. temperature range of the HgTe-like (T_0-mode) and CdTe-like (T_1-mode) sub-band maxima on the Im[ε(ω,T)] curves $Hg_{1-x}Cd_xTe$ (x=0.11)





E.M. Sheregii, at al., *PRL* **102,** 045504, (2009)

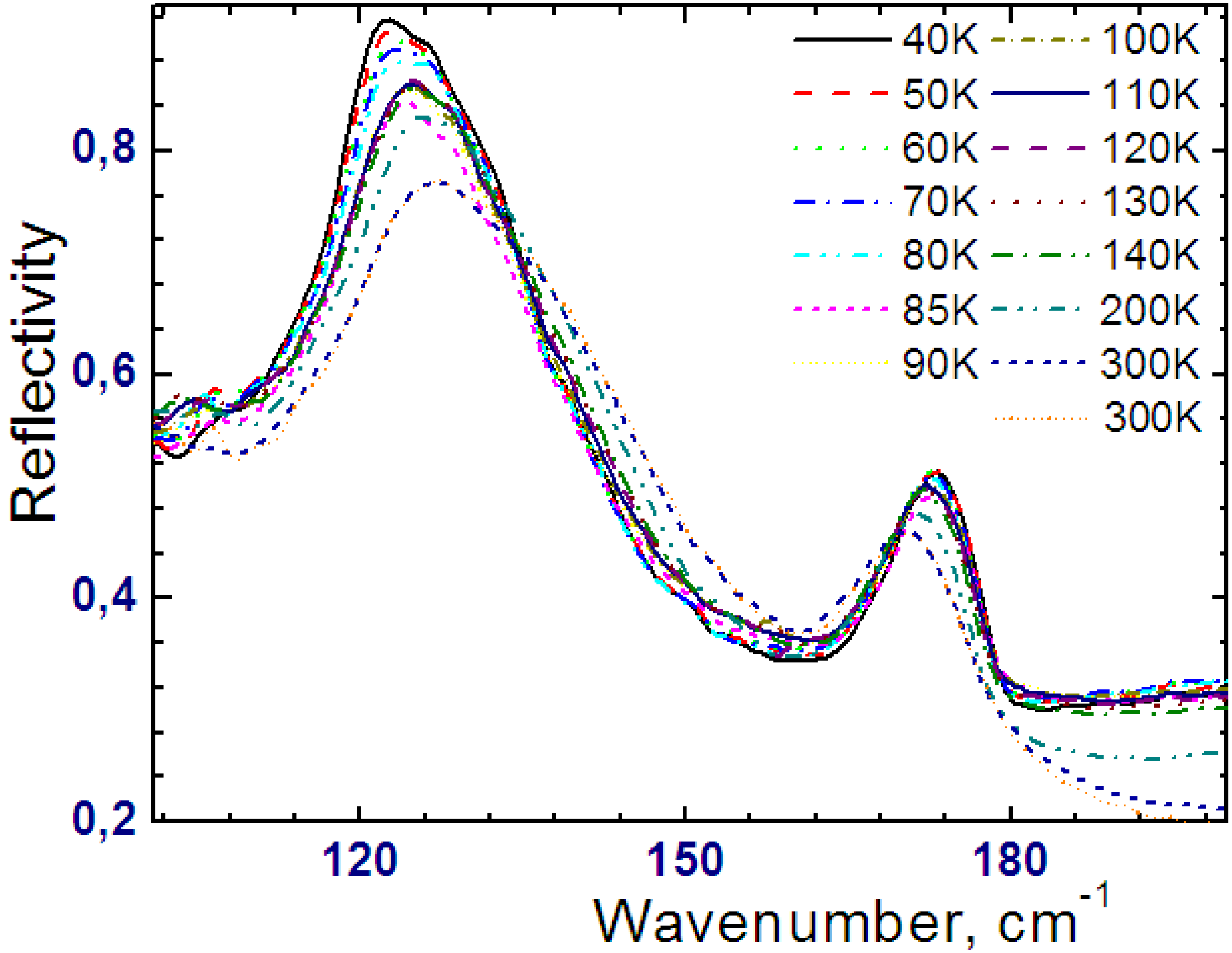
$$\omega_{TO}^{*2} = \omega_{TO}^{2} \pm \frac{4\,\Xi_{CV}^{2}}{Ma^{2}W}\ln\frac{W}{2E_F + |E_g|}$$

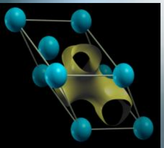


The optical reflectivity experiment

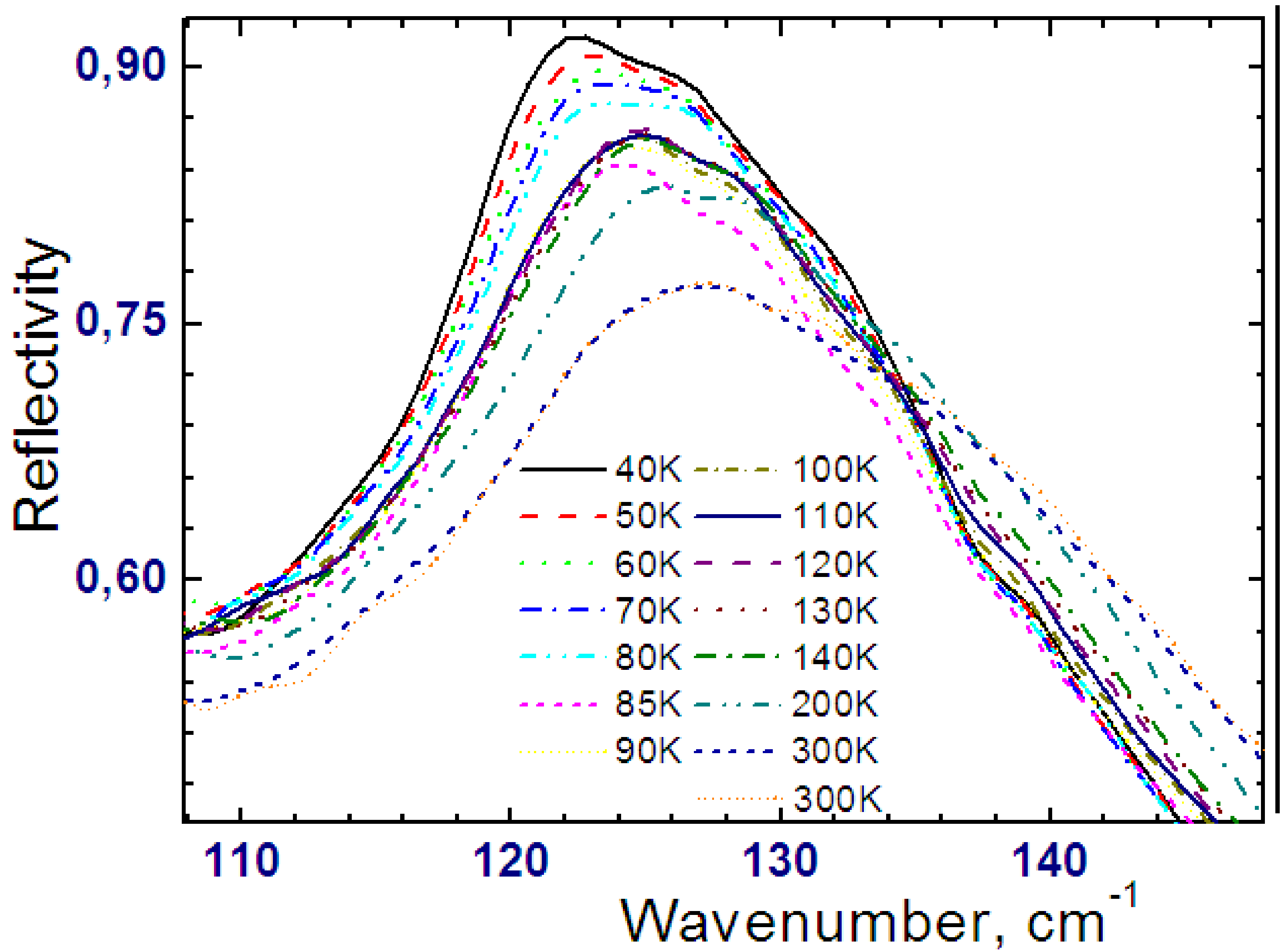
in the far-infrared region

$Hg_{1-x}Zn_xTe$ $(x=0.06)$





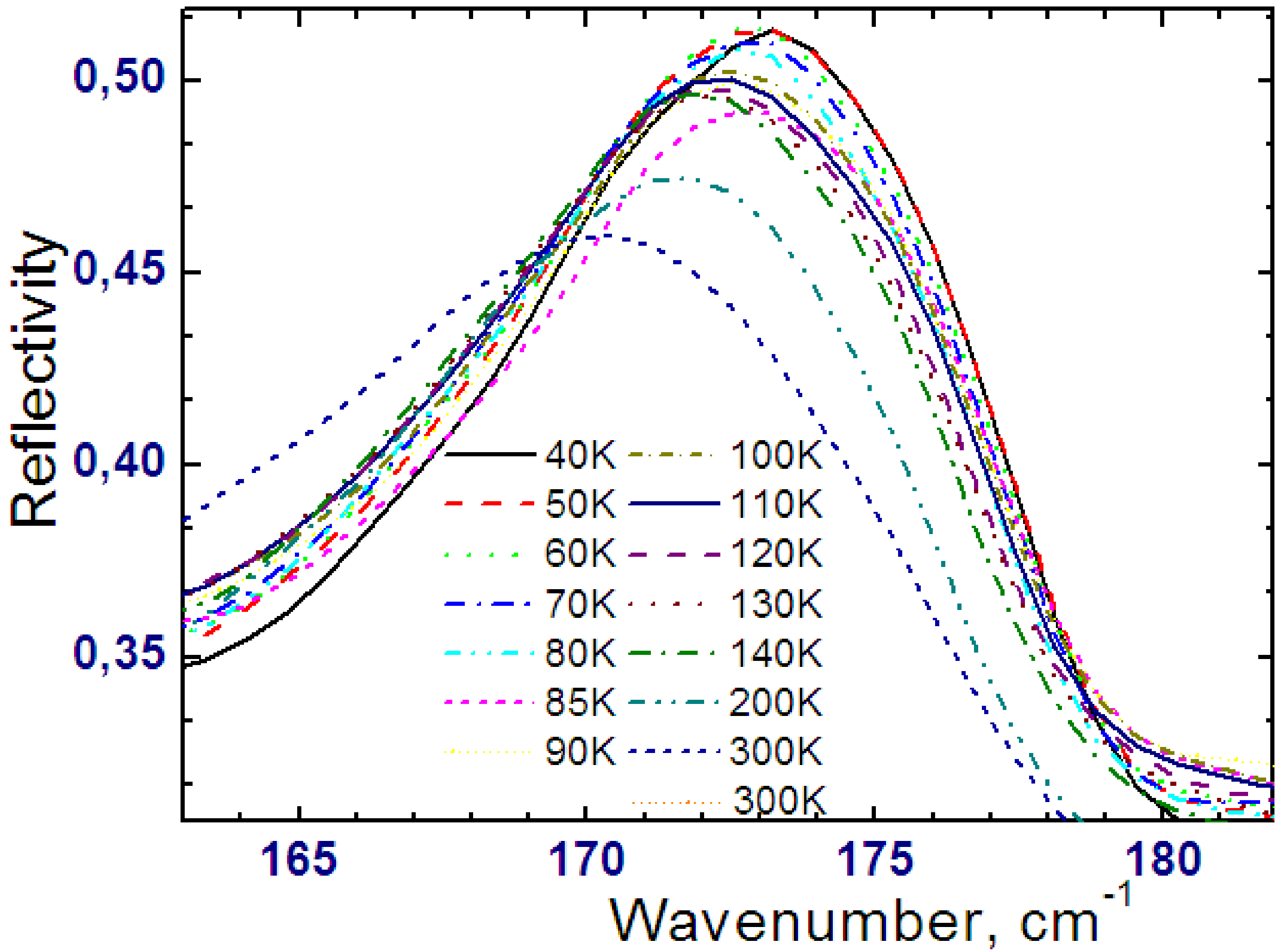
The optical reflectivity experiment
in the far-infrared region



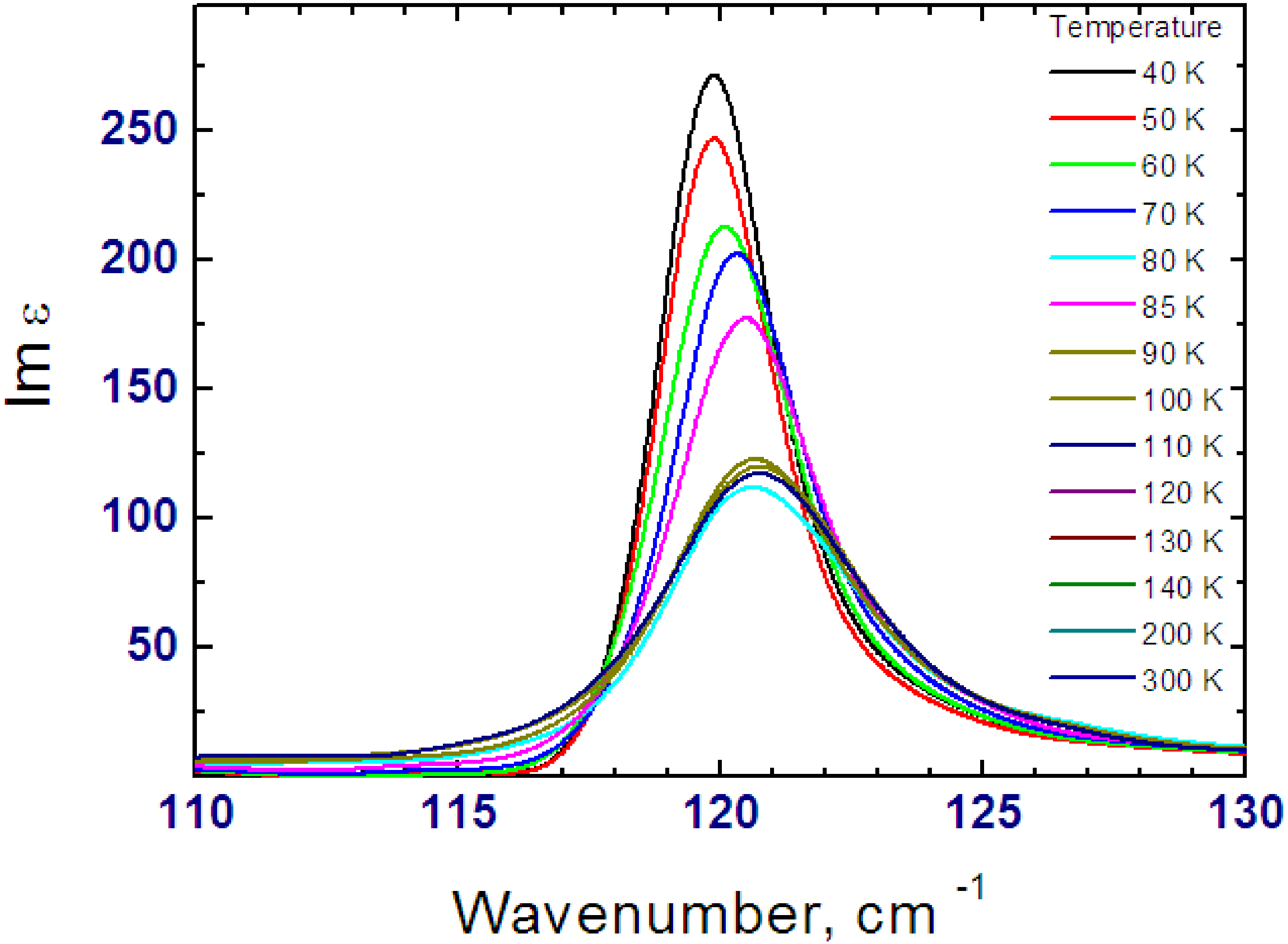
The optical reflectivity experiment

in the far-infrared region

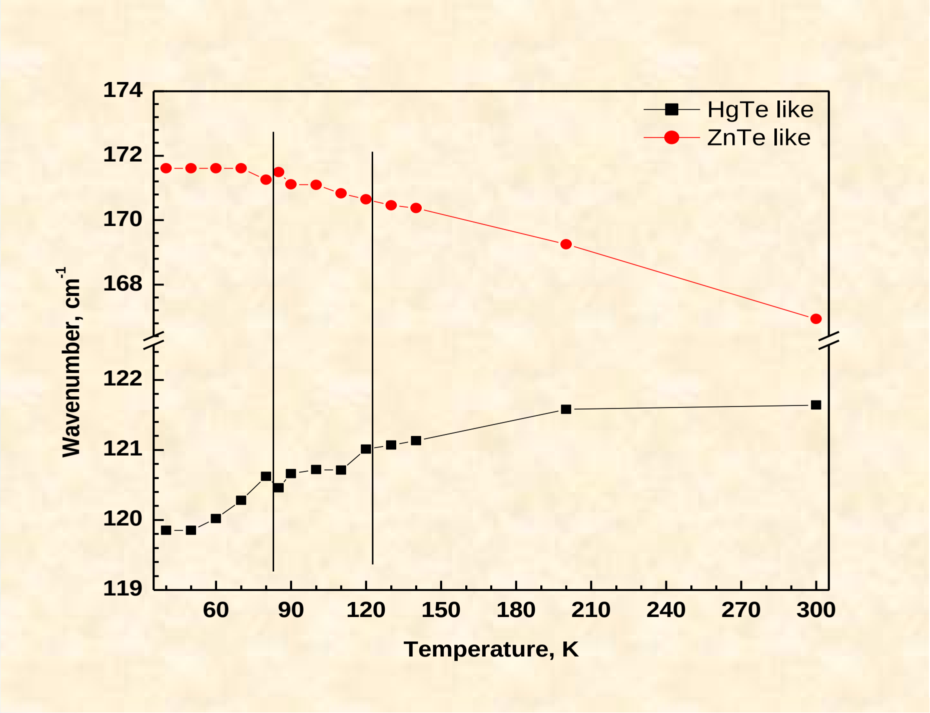
$Hg_{1-x}Zn_xTe$ (x=0.06)

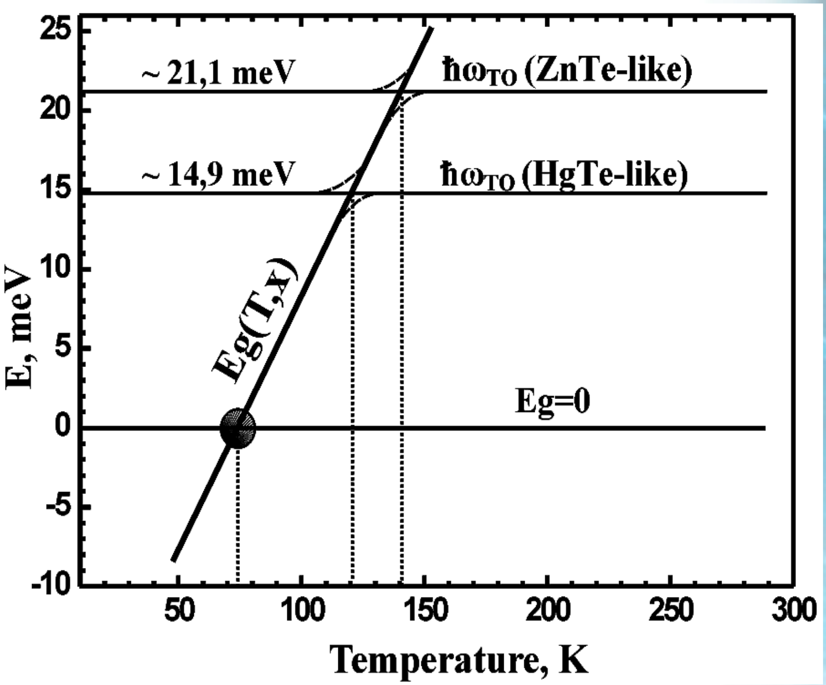


The dielectric function
imaginary part, HgTe-like sub-band
$Hg_{1-x}Zn_xTe$ (x=0.06)



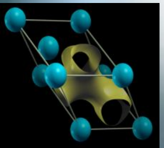
The frequency positions vs. temperature range of the HgTe-like (T_0-mode) and ZnTe-like (T_1-mode) sub-band maxima on the Im[ε(ω,T)] curves $Hg_{1-x}Zn_xTe$ (x=0.06)





SUMMARY

- Experimental data of the optical reflectivity for $Hg_{1-x}Cd_xTe$ (x=0.115) and $Hg_{1-x}Zn_xTe$ (x=0.06) samples) obtained in a wide interval of temperature (from 20 K to 290 K) and in the far-infrared (FIR) domain with using a brilliant synchrotron radiation show that frequencies of the optical phonon modes exhibit discontinuity in their temperature dependence when a **zero-gap state occurs**.
- This discontinuity is evidence of the **returnable electron-phonon coupling** in semiconductors.
- **The mechanism of returnable electron-phonon coupling is deformation potential** not polar one.



Acknowledgments

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Thank you for your attention