

 $44.30.+v$ Heat transfer in inhomogeneour media and through interfaces

Noise (turbulence generated)

47.25.gv

 $47.90.+a$ Other topics in fluid dynamic

γ sics and As Physics and Astronom₎
Classification Scheme -

GENERAL

philosophy

and fields

physics

01.Communication, education, history, and

05.Statistical physics and thermodynamics 06.Measurement science, general laboratory techniques, and instrumentation systems 07.Specific instrumentation of general use in

02. Mathematical methods in physics 03.Classical and quantum physics; mechanics

THE PHYSICS OF ELEMENTARY PARTICLES AND FIELDS

23. Nuclear decay and radioactivity 24. Nuclear reactions and scattering: general 25. Nuclear reactions and scattering: specific

particle systematics

resonances

reactions

ranges

studies

NUCLEAR PHYSICS 21.Nuclear structure

11.General theory of fields and particles 12. Specific theories and interaction models:

13.Specific reactions and phenomenology 14.Properties of specific particles and

04. Relativity and gravitation

(ICSU/AB International Classification for Physics)

American Institute of Physic

335 East 45th Stree

New York, N.Y. 100 335 East 45th Street New York, N. Y. 10017

Indexing articles for physics journals

With the exceptions of Sections 84, 85, and 89 and the fine detail listed in the Appendices, the scheme presented here is the 1977 International Classification for Physics agreed upon for 1977 by the member services of the Abstracting Board (Physics Working Group) of the International Council of Scientific Unions. The hope is that physicists and other users of physics information will eventually encounter only this one common classification scheme in the widest possible spectrum of publications and services.

In the alphanumeric codes printed here the last character (a lower case letter) is a check digit, which can be computed from the previous characters by a predetermined algorithm. This algorithm is incorporated in the computer programs used by AIP for the production of journal indexes, so that illegitimate code assignments (resulting from typing errors, for example) can be detected and flagged.

In using this scheme to index an article, please observe the following rules:

- Always include the check character
- ~ pick no more than four index codes
- ~ designate one of these as the principal index code by placing it first in your list
- ~ always choose the lowest-level code available.
- avanaore.
(Third-level codes ending in a "+" sigr do not have further sublevels, but do not nave further subfevers, but
those ending in a "-" sign do have sublevels and should only be used if none of the fourth-level codes are appropriate or general enough. Please, examine all the headings at a given level, noting that in cases of apparent overlap the headings are intended to be mutually exclusive, and choose those headings that best seem to fit the substance of your paper.)

We would appreciate any comments or suggestions you may have, both on the scheme and the form of presentation. Please address them to the Editor of the journal for which you are indexing or to one of the undersigned.

Samuel Schiminovich, PACS Editor A.W. Kenneth Metzner, Director, Publications Division

Summary of Scheme

CONDENSED MATTER: STRUCTURE
MECHANICAL AND THERMAL PROPERTIES

- 61.Structure of liquids and solids; crystallography
- 62.Mechanical and acoustical properties of condensed matter
	- 63.Lattice dynamics and crystal statistics
	- 64. Equations of state, phase equilibria, and phase transitions
	- 65.Thermal properties of condensed matter
	- 66.Transport properties of condensed matter (nonelectronic)
	- 67.Quantum fields and solids; liquid and solid helium
	- 68.Surfaces and interfaces; thin films and whiskers

CONDENSED MATTER: ELECTRONIC STRUCTURE, ELECTRICAL, MAGNETIC, AND OPTICAL PROPERTIES

- 71.Electron states
- 72. Electronic transport in condensed matter
- 73. Electronic structure and electrical properties
- of surfaces, interfaces, and thin films
- 74.Superconductivity
- 75.Magnetic properties and materials
- 76.Magnetic resonances and relaxation in condensed matter: Mössbauer effect
- 77.Dielectric properties and materials
- 78.Optical properties and condensed-matter spectroscopy and other interactions of matter with particles and radiation
- 79.Electron and ion emission by liquids and solids; impact phenomena

RELATED AREAS OF SCIENCE AND
TECHNOLOGY

- 81.Materials science
- 82.Physical chemistry
- "84.Electromagnetic technology
- "85.Electrical and magnetic devices
- 87.Biophysics, medical physics, and biomedical engineering
- "89.Other areas of research of general interest to physicists

G EOPHYSICS, ASTRONOMY, AND **ASTROPHYSICS**

- 91.Solid Earth geophysics
- 92.Hydrospheric and atmospheric geophysics
- 93.Geophysical observations, instrumentation,
- and techniques
- 94.Aeronomy and space physics 95.Fundamental astronomy and astrophysics; instrumentation, techniques, and
	- astronomical observations
- 96.Solar system
- 97.Stars
- 98.Stellar systems; galactic and extragalactic objects and systems; The Universe

"APPENDICES

- 02. Mathematical methods in physics
- 43.Acoustics

*These Sections are outside the ICSU/AB International Classification for Physic

CLASSICAL AREAS OF PHENOMENOLOGY (INCLUDING APPLICATIONS)

- charged particles 42.Optics
-
- processes
- 47. Fluid dynamics
- FLUIDS, PLASMAS, AND ELECTRIC **DISCHARGES**
- 51.Kinetic and transport theory of fluids; physical properties of gases
- 52.The physics of plasmas and electric

- 29. Experimental methods and instrumentation for elementary-particle and nuclear physics
- theory

27. Properties of specific nuclei listed by mass

28. Nuclear engineering and nuclear power

- photons
- molecules with photons
- 34.Atomic and molecular collision processes and interactions
- 35.Experimentally derived information on atoms and molecules; instrumentation and techniques
- 36.Studies of special atoms and molecules

-
-
- 44. Heat flow: thermal and thermodynamic
-

ATOMIC AND MOLECULAR PHYSICS

- 31. Electronic structure of atoms and molecules, CROSS-DISCIPLINARY PHYSICS AND
- 32.Atomic spectra and interactions with
- 33. Molecular spectra and interactions of
-
-
-
-
-
- 41.Electricity and magnetism: fields and
-
- 43.Acoustics

46.Mechanics, elasticity, rheology

-
-
- discharges

02.20.+^b Group theory (for algebraic methods in quantum mechanics, see 03.65.F; for symmetries in elementary particle physics, see 11.30)

 $02.30.+g$ Function theory, analysi

00. GENERAL

 $\overline{\mathbf{I}}$

 $\,$ ii

 $05.90 + m$ Other topics in statistical

- $06.90.+v$ Other topics in measurement science, general laboratory techniques and instrumentation systems
- 07. Specific instrumentation and techniques of general use in physics (see also within each subdiscipline for specialized instrumentation and techniques)
- $07.10.+i$ Mechanical instruments and measurement methods
- 07.20. n Thermal instruments and techniques $07.20.Dt$ Thermometry
- 07.20 . Fw Calorimetry 07.20.Hy $\ensuremath{\mathsf{F} \mathsf{urnaces}}$ 07.20 .Ka High-temperature techniques and instrumentation; pyrometry 07.20.Mc Cryogenics
- $07.25.+f$ Hygrometry
- $07.30 t$ Vacuum production and techniques (see also 47.45. Rarefied gas dynamics, 47.80. Fluid dynamics instrumentation) 07.30.Bx Evacuating power, degasification, residual gas 07.30.Cy Vacuum pumps $07.30 \text{ D}z$ Vacuum meters 07.30.Hd Vacuum apparatus and testing methods $07.30.Kf$ Auxiliary apparatus, hardware, and materials $07.35.+k$ High-pressure production and techniques $07.50.+f$ Electrical instruments and techniques $07.55 + x$ Magnetic instruments and
- techniques
- $07.58.+g$ Magnetic resonance spectrometers, auxiliary instruments, and techniques (see also 61.16.H. EPR and NMR determinations)

10. THE PHYSICS OF ELEMENTARY PARTICLES AND FIELDS (FOR COSMIC RAYS, SEE 92; FOR EXPERIM. METHODS AND INSTRUMENTATION, SEE 29)

Servo and control devices

Transducers

 $06.70 Mx$

06.70.Td

Other topics in specialized

instrumentation

 $07.90.+c$

12. Specific theories and interactio models; particle systematic

21. Huclear structure

20. NUCLEAR PHYSICS

For hadronic atoms and molecules, see 36.10.G

 $21.80.+a$ Hypernucl $21.90.+f$ Other topics in nuclear structur

23. Nuclear decay and radioactivit (see also 82.55. Radiochemistr

23.90.+w Other topics in nuclear decay and radioactivity

25.30.Cg 25.30.Ei 25, 30.Gk scattering

Muon scattering Neutrino scattering

Electron and positron scattering

27.90. + b $220 \le A$

30. ATOMIC AND MOLECULAR PHYSICS (FOR PHYSICAL CHEMISTRY, SEE 82)

 $\overline{1}$

33.70.Ca Oscillator and band strengths, transitio
moments, and Franck–Condon factors

35. Experimentally derive information on atoms and molecules; instrumentation and techniques

40. CLASSICAL AREAS OF PHENOMENOLOGY (INCLUDING APPLICATIONS)

 $42.90.+m$ Other topics in optics

50. FLUIDS, PLASMAS, AND ELECTRIC DISCHARGES (FOR FLUID DYNAMICS, SEE 45; FOR CONDENSED MATTER, SEE 60 AND 70)

52.25.Mq Dielectric properties 52.25.Ps Emission, absorption, and scattering of radiation

 $of\,$

60. CONDENSED MATTER: STRUCTURE, **MECHANICAL AND THERMAL PROPERTIES**

scattering

For acoustoelectric effects, see 72.50

TO. CONDENSED MATTER: ELECTRONIC STRUCTURE, ELECTRICAL, MAGNETIC, AND OPTICAL PROPERTIES

73.40.Mr

 $7₃$

 $\overline{7}$

74,30.Gn

Response to electromagnetic fields,
nuclear magnetic resonance, ultrasor
attenuation

 $\bf 78.$

 $78.20.\mathrm{Ek}$

 78.20 ${\rm Fm}$

78.20.Hp

 $78.20.Jq$

 $78.20.Ls$

 78.20 \rm{Nv}

78.30.Cp

 $78.30\!\cdot\!{\rm Er}$

Optical rotatory power

Electro-optical effects

Magneto-optical effects

Thermo-optical effects $78.30. - j$ Infrared and Raman spectra and

 $_{\rm effects}$

 $scattering$

Birefringence (including stress
birefringence, flow birefringence, etc.)

Infrared and Raman spectra in liquids

Infrared and Raman spectra in metals

Piezo-, elasto-, and acousto-optical

79. Electron and ion emission by liquids and solids; impact phenomena

80. CROSS-DISCIPLINARY PHYSICS AND RELATED AREAS OF SCIENCE AND TECHNOLOGY

81. Materials science

82. Physical chemistry

$82.20 - w$ Chemical kinetics 82.20.Db Statistical theories, including transition state 82.20.Fd Stochastic and trajectory models, other theories and models 82.20.Hf Mechanisms and product distribution Potential energy surfaces for chemical 82.20.Kh reactions (see also 31.70.F. —in atomic
and molecular physics; 34.20.B.
General potential functions, 34.50.L. Chemical reactions, as studied by
atomic and molecular beams) 82.20.Mj Nonequilibrium kinetics 82.20.Pm Measurements of rate constants, reaction cross sections, and activation energies 82.20.Rp Energy distribution and transfer;
relaxation (see also 31.70.H. Timedependent phenomena -in atomic and molecular physics 82.20.Tr Kinetic and isotope effects $82.20.\mathbf{W}t$ Computational modeling

 $84.$

90. GEOPHYSICS, ASTRONOMY, AND ASTROPHYSICS

91.50.Ey Ocean bottom processes

91. Solid Earth geophysics

For atmospheric optics, see 42.68

 $92.90.+x$ Other topics in hydrospheric and atmospheric geophysics

93. Geophysical observations,
instrumentation, and techniques

 $91.50.Cw$

Beach, coastal, and shelf processes

97. Stars

ERRATA

Special instruction: for "Errata" items use 99.10.+g in
addition to all the codes assigned to
the original article.

Kaufmann, L. R. Medsker, J. W. Nelson, and R. G. Flocchini, Phys. Rev. Lett. 37, 11 (1976).

 2 In contrast to his former information, Gentry recently informed us that the monazite samples (M1) are from the same ore body, but more than 10 km away from where the biotite with giant halos have been found.

 $3J.$ D. Fox, W. J. Courtney, K. W. Kemper, A. H.

Lumpkin, N. R. Fletcher, and L. R. Medsker, Phys. Rev. Lett. 37, 629 (1976).

'L. K. Peker, V. M. Sigalov, and Yu. I. Kharitonov, Nucl. Data Sheets 12, 343 (1974).

 $5J$. W. Nelson, private communication.

 $6A$ more detailed account of our investigations will be published elsewhere.

Commensurate Ordering in Tetrathiafulvalene-Tetracyanoquinodimethane

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Institute of Physics of the University, Zagreb, Croatia, Yugoslavia (Received 14 July 1976)

Is is suggested that the first-order instability in tetrathiafulvalene-tetracyanoquinodimethane $[(TTF)-(TCNQ)]$ at 38 K is related to the fourth-order umklapp coupling which concerns the wave vectors of the star involved in the three-dimensional periodic ordering. Within the anharmonic TCNQ interchain-coupling model, we predict that the configuration of chain deformation changes abruptly at 38 K, provided that this coupling is attractive.

The recent structural investigations' on (TTF)- (TCNQ) have revealed the existence of a peculiar three-dimensional ordering of the Peierls deformations $(q_b = 0.295b^*)$ in the temperature range between 54 and 38 K.

Between 54 and 49 K, the most unstable wave vector has a component in the direction of alternating chains equal to $a*/2$; below 49 K, this component starts to decrease. This effect was thoroughly discussed in the recent work by Bak and Emery,² where it was attributed to the bilinear coupling of the intrinsically different Peierls deformations on TCNQ and TTF chains. A similar explanation was also mentioned. but only briefly, in an earlier paper by Saub, Barisic, and Friedel.³ Here we accept such an interpretation of the 54-K and 49-K transitions, but for the third transition at 38 K we wish to suggest an alternative explanation to that proposed in Ref. 2.

At 38 K, q_a jumps to the commensurate value $q_e = a^*/4$ and remains pinned to this value at lower temperatures. In Ref. 2, this effect was attributed to the fourth-order umklapp coupling in which the $(a*/4, q_h)$ wave on TCNQ chains, taken to the third power, is umklapp-coupled to the $(a*/a)$ 4, $-3q_b$) wave of the TTF chains. However, the full crystal symmetry also allows the fourth-order umklapp coupling of the waves involved in the star $(\pm a^*/4, \pm q_h)$ [Fig. 1(a)]. In principle, four coupled waves can belong either to TCNQ or to TTF chains and mix together in the fourth-order invariants. Obviously, this alternative does not imply any additional scattering at 38 K such as that expected at $-3q_b=0.115b^*$ for the mechanism

of Ref. 2.

We have performed the actual calculations in the model which retains only the coupling of the

FIG. 1. (a) The star of wave vectors $(\pm q_a, \pm q_b)$. (b) The phase-shift chain deformations corresponding to the solution with only two waves ψ_1 , ψ_1^* being different from zero. (c) The "amplitude-wave" configuration involving all four waves in the star with the same amplitude.

four large TCNQ waves. It will appear that the $interchain$ coupling of the TCNQ waves governs the pinning effect at 38 K. This limits our model to the situations in which the strength of the TCNQ deformation compensates for the fact that the anharmonic coupling constant for the TCNQ interchain coupling is probably smaller than for the TCNQ-TTF coupling. The mixed terms are not expected to change essentially our conclusions at 38 K, but they would affect⁴ the Peierls instability in the particular chain family and the sliding behavior of q_a . There is, however, no strong experimental evidence that this happens in (TTF)-(TCNQ), where the bilinear TCNQ- TTF coupling alone explains the 54-38K temperature range.

Using the notations defined in Fig. $1(a)$, the fourth-order terms involving TCNQ chains for q_a < $a^*/2$ are

$$
\frac{b_1(\rho_1^4 + \rho_2^4) + b_2'\rho_1^2\rho_2^2}{\left[\frac{-a}{(2b_1 + b_2')}\right]^{1/2}} \cdot \frac{(1)}{\cos\left(q_b\right)b + \frac{\theta_1 - \theta_2}{2}\right)\cos\left(q_ana + \frac{\theta_1 + \theta_2}{2}\right)},
$$
\n(3)

shown on Fig. $1(c)$. In contrast to the first case, the chain waves are not shifted relatively one to another, but instead, the amplitude depends periodically (with the period $2\pi/q_a$) upon the chain index n .

In Eqs. (2) and (3) we distinguish the phases θ , or $(\theta_1-\theta_2)/2$ associated with the incommensurate wave number q_b and the phase $(\theta_1 + \theta_2)/2$ which in the "amplitude wave" goes with the potentially commensurate wave number q_a . When $q_a = a^*/4$, this phase appears in the fourth-order deformation energy (1). This is the lowest-order phasedependent term built by the star of Fig. $1(a)$, i.e., there is no third-order invariant of such a nature,

The minimization of Eq. (1) with respect to θ , + θ_2 gives $b_2' = b_2 - 2|b_3|$ and $\theta_1 + \theta_2$ equal to $\pi/2$ (for $b_3 > 0$) or to 0 (for $b_3 < 0$). The condition $|b_{2}|/2b_{1}$ < 1 established above for the stability of the "amplitude wave" (ii) thus becomes at 38 K the condition for the pinning of q_a on $a^*/4$, [i.e., $|b_{2}-2|b_{3}|$ $|<$ 2b₁]. When the fourth-order contributions are written in terms of displacements instead of the order parameters $\psi_{1,2}$, this condition amounts to the requirement that the fourthorder interchain interaction is attractive. If so, the configuration of TCNQ waves at 38 K is that of Fig. 1(c), with the amplitudes of waves equal to 2 $[-2a/(2b_1+b_2-2|b_3|)]^{1/2}$ (for $b_3 > 0$), or to 0 and $4\left[-a/(2b_1+b_2-2|b_3|)\right]^{1/2}$ (for $b_3<0$).

where

$$
b_2' = b_2 + 2b_3 \delta_{q_a, a^* / 4} \cos 2(\theta_1 + \theta_2).
$$
 (1a)

In general the coefficients $b_{1,2,3}$ are independent. The umklapp, phase-dependent b_3 term favors, under conditions determined below, the Peierls deformation with $q_a = a^*/4$.

The system with the anisotropic anharmonic energy (1) is stable for $b_1 > 0$, $b_2' / 2b_1 > -1$. Two different deformation configurations are then possible regarding the value of ratio $b_2'/2b_1$: (i) For $b_2'/2b_1 > 1$, the Landau-Ginzburg energy is mini- $\frac{\partial_2}{\partial_1}$ the Landau-Ginzburg energy is missimal for $\rho_1 = 0$, $\rho_2 = (-a/2b_1)^{1/2}$ (or vice versa) where $a \equiv a'(T - T_{\odot})$ and $T_{\odot} = 54$ K. The deformation on *j*th place in *n*th chain is equal to

$$
2(-a/2b_1)^{1/2}\cos(q_b j b + q_a n a + \theta_1), \qquad (2)
$$

and is shown on Fig. 1(b). q_a represents here the phase shift of the two neighboring chain waves with equal amplitudes. (ii) For $|b_2'|/2b_1 < 1$, ρ_1 with equal amplitudes. (ii) F or $\frac{p_2}{2}$ $\frac{p_1}{2}$, $\frac{p_1}{p_2}$ = $\frac{p_2}{2}$ = $\left[-\frac{a}{2b_1 + b_2} \right]^{1/2}$. This solution leads to the deformation

$$
(3)
$$

It remains for us to find out which of the two configurations shown in Figs. $1(b)$ and $1(c)$ is present in (TTF)-(TCNQ) between 54 and 38 K. For this purpose, we use the experimental fact that no discontinuity is observed in the TCNQ deformation in the temperature range 38 K $\lt T$ $<$ 54 K.¹ This range includes the temperature T =49 K at which q_a starts to decrease from $a*/2$. For $q_a = a^*/2$ [i.e., at temperatures 49 K < T < 54 K , the star of Fig. 1(a) reduces to only two independent components $\psi_{\pm\pi} = \rho_{\pi} \exp(\pm i\theta_{\pi})$. The fourth-order invariant is then of the form $b_{\pi}\rho_{\pi}^4$. With the equilibrium value $\rho_{\pi} = (-a/2b_{\pi})^{1/2}$, the deformation is

$$
2(-a/2b_{\pi})^{1/2}\cos(q_{b}jb+n\pi+\theta_{\pi}).
$$
\n(4)

We can compare the amplitude of the deformation (4) and the related deformation energy at 49 K with the corresponding quantities of configura-
with the corresponding quantities of configurations (i) and (ii). The conclusion is that only the transition from the configuration (4) to the configuration (i) can be continuous, and it is provided that $b_{\pi} = b_{1}$. Thus in our model and in the temperature range 38 K < T < 49 K, the equivalent configurations $\{\rho_1 \neq 0, \rho_2 = 0\}$ [Fig. 1(b)] and $\{\rho_1 = 0, \rho_2\}$ $\neq 0$ are associated with the lowest-order free energy $(b_2 > 2b_1)$.⁵ On a macroscopic scale, we would expect equal proportion of domains with

these two structures.

The overall prediction of the present model for the first-order instability at 38 K is that, besides the discontinuity in the amplitude of chain waves, it involves the transition from the configuration with the phase shift $[Fig. 1(b)]$ to the essentially different configuration with the "amplitude wave" in the a direction.

Our final remark concerns the excitations at and below 38 K. In the usual picture the terms of the type b_3 in Eq. 1(a) are included into the sine-Gordon equation for the phase. This leads to the soliton solution: The phase is $(q_a na +cte)$ in large regions of the crystal; these regions are separated by walls where the phase changes abruptly by the amount $2\pi/M = \pi/2$. Our feeling is that the situation is in fact more complicated, because the phase differs from $(q_a na +cte)$ in the wall and, according to Eq. 1(a), the cosine term switches off there. The question of excitations seems

therefore to require further investigation, based perhaps on the continuity of the umklapp terms in the unaveraged energy.

We gratefully acknowledge clarifying discussions with R. Comes, J. R. Cooper, and J. A. Krumhansl.

¹R. Comes, S. M. Shapiro, G. Shirane, A. F. Garito, and A. J. Heeger, Phys. Rev. Lett. 35, 1518 (1975), and to be published; see also the pioneering work by D. Jerome, W. Muller, and M. Weger, J. Phys. (Paris), Lett. 35, 77 (1974).

 2 Per Bak and V. J. Emery, Phys. Rev. Lett. 36, 978 (1976).

 3 K. Saub, S. Barisić, and J. Friedel, Phys. Lett. 56A, 302 (1976).

 ${}^{4}E.$ g. I. F. Lyuksyutov, Phys. Lett. 56A, 135 (1976). 5 The same conclusion can be drawn from the model of the predominantly local (intrachain) fourth-order coupling.