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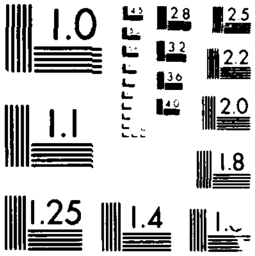
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CUMENTATION PAGE

Form Approved
OMB No 0704-0188
Exp Date Jun 30, 1986

1a. REPORT SECURITY CLASSIFICATION
Unclassified

1b. RESTRICTIVE MARKINGS

2a. SECURITY CLASSIFICATION AUTHO

2b. DECLASSIFICATION / DOWNGRADI EDULE

3. DISTRIBUTION / AVAILABILITY OF REPORT
Approved for public release; distribution unlimited.

4. PERFORMING ORGANIZATION REPORT NUMBER(S)

5. MONITORING ORGANIZATION REPORT NUMBER(S)
R&D 5181-EE-01

6a. NAME OF PERFORMING ORGANIZATION
University of Graz

6b. OFFICE SYMBOL *(If applicable)*

7a. NAME OF MONITORING ORGANIZATION
USARDSG-UK

6c. ADDRESS *(City, State, and ZIP Code)*
Institut fur Theoretische, Universitatsplatz
5, Graz, Austria

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Box 65
FPO NY 09510-1500

8a. NAME OF FUNDING / SPONSORING ORGANIZATION
USARDSG-UK

8b. OFFICE SYMBOL *(If applicable)*

9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
DAJA45-85-C-0048

8c. ADDRESS *(City, State, and ZIP Code)*
Box 65
FPO NY 09510-1500

10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO
61102A	1L161102BH57	03	

11. TITLE *(Include Security Classification)*
Submicron Phonoics II

12. PERSONAL AUTHOR(S)
Professor P. Kocevar

13a. TYPE OF REPORT
Final

13b. TIME COVERED
FROM 1985 TO 1987

14. DATE OF REPORT *(Year, Month, Day)*
87.12.30

15. PAGE COUNT
8

16. SUPPLEMENTARY NOTATION

17. COSATI CODES

FIELD	GROUP	SUB-GROUP

18. SUBJECT TERMS *(Continue on reverse if necessary and identify by block number)*
(U) Phonon, ~~(U)~~ Phonon-Electron Interaction, ~~(U)~~ Device Modelling, ~~(U)~~ Non-Equilibrium Phonon Model, (U) Semiconductor Transport

19. ABSTRACT *(Continue on reverse if necessary and identify by block number)*

Results to implement non-equilibrium phonon distributors into a conventional Monte Carlo electron transport simulation are report. A new code for a simulation of the simplified model of low-tempreature steady-state acoustic phonon-electron transport in GaAs has been developed and applied. This model has been extended to a fully time-dependent (transient) calculation of optical @honon interactions with near ballistic electrons in n-GaAs in the overshoot regime at room temperature (1) by modifying standard Monte Carlo codes to accommodate the numerical procedures required for nonequilibrium phonon calculations and by applying these to real device phenomena such as picosecond response in n-GaAs to a high field pulse.

20. DISTRIBUTION / AVAILABILITY OF ABSTRACT
☒ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☒ DTIC USERS

21. ABSTRACT SECURITY CLASSIFICATION
Unclassified

22a. NAME OF RESPONSIBLE INDIVIDUAL
Dr. John M. Zavada

22b. TELEPHONE *(Include Area Code)*
01-409 4423

22c. OFFICE SYMBOL
AMXSN-UK-RI

DD FORM 1473, 84 MAR

83 APR edition may be used until exhausted.
All other editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE

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Graz, December 30, 1987

FINAL REPORT

(Contract Nr. DAJA 45-85-C-0048)

Project: SUBMICRON PHONONICS II

1. The Problematics of Phonon Disturbances in D.C.Semiconductor Transport

Since the early days of modern solid-state theory phonon disturbances have been discussed in connection with fundamental aspects of charge transport. Peierls (1930) and later Klemens (1951) had recognized their importance and in particular the essential role of nonelectronic relaxation processes of the *nonequilibrium phonons for the establishment of a steady state of the coupled carrier-phonon system* in the presence of a d.c. electric field. Contributions of mutual drag effects between carriers and phonons to the electrical and thermal conductivity and to the thermopower of semiconductors were first estimated by Sondheimer and Parrot(1956,1957), who also pointed out that the neglect of phonon disturbances in the calculation of electronic transport coefficients leads to a violation of the Onsager and Kelvin relations. It is interesting to note that even in the ohmic *case any drag effect of nonequilibrium phonons on the electrons* introduces a nonlinear current-field characteristics, because the phonon distributions and therefore the rates for carrier-phonon scattering become field dependent, in contrast to the linear-response concept of field- independent electronic mobilities. But the most practical aspects of phonon disturbances concern the nonlinear response phenomena connected with high-field transport and laser-pulse excitation of semiconductors.

Because of the weak carrier-phonon couplings and of the rapid increase of the thermalisation rate of acoustic modes with temperature, possible mobility effects of acoustic-phonon disturbances are restricted to lattice temperatures of at most a few degrees K. At these temperatures the great difficulties in the treatment of the dominant ionised-impurity scattering overshadow the question about possible nonequilibrium-phonon *effects on the theoretical carrier mobilities, but phonon-drag-induced increases* of the mobility by more than 20 percent have been found in simple model calculations (Kocevar and Fitz 1977,1978).

In contrast to the acoustic case, the dependence (i.e. *increase*) of the thermalisation rates of optical phonons with temperature is only weak. Although these rates are very fast, of the order of inverse picoseconds, the strong polar optical carrier-LO-phonon coupling in polar materials can lead to even faster emission rates of phonons by the carriers and therefore to substantial LO-phonon amplification even at room temperature.

The practically most interesting candidate among the standard semiconductors for noticeable mobility effects of such nonequilibrium LO phonons is n-GaAs, where the time constants for valley-transfer and for the generally expected ensuing velocity overshoot are again in the picosecond range and therefore comparable to the above discussed time constants for the buildup of phonon disturbances. Since the phonon amplification *acts back on the carrier distribution and modifies the carrier populations* of the different valleys, the question arises whether there might be interference effects between the phonon buildup and the performance of high-speed GaAs devices designed to work in the velocity-overshoot regime.

The preceding research project "Submicron Phononics I", Contract Number DAJA45-84-M-0394, had been set up to provide a first step towards a quantitative estimate of such transient nonequilibrium phonon effects in GaAs devices by implementing phonon disturbances into the conventional Displaced-Heated-Maxwellian (HDM) carrier models of nonlinear transport.

The physical model used in the preceding as well as in the present research project consists of electrons in isotropic and parabolic Γ- and L-conduction band minima with the standard electron-phonon couplings: polar optical, inequivalent and equivalent intervalley, acoustic deformation potential, optical deformation potential (L-valley), piezoacoustic (not contained in the Monte Carlo model), and ionised impurity scattering. The model assumes *spatial* homogeneity, neglecting *in particular the very small* LO-phonon diffusion, but should nevertheless allow its extrapolation to a coarse-grained and therefore locally homogeneous description of space-dependent situations.

The results of "Submicron Phononics I" could be summarised as follows:

(1A) *Neglecting the upper L-valleys, a nonequilibrium-phonon-induced collective breakdown occurs* within the typical field and time range of the overshoot effect in the actual many-valley bandstructure. The breakdown is caused by an LO phonon avalanche through a "Phonon-Cerenkov" mechanism (i.e. the mean carrier drift velocity must exceed the phase velocity of the phonons) and requires a sufficiently high carrier concentration. As the mathematical resonance condition is a consequence of the HDM distribution of the carriers, the model dependence of this prediction is obvious, but a Cerenkov-like phonon amplification should be expected, whenever the actual carrier distribution is of HDM form.

(1B) For the realistic many-valley bandstructure it turns out that the loss of fast-drifting Γ-electrons through transfer into the "slow" L-valleys suffices to stop the above mentioned single-valley breakdown and to *ensure the establishment of an asymptotic steady state* at arbitrary fields. Carrier drag by the initially amplified forward phonons dominates at fields below the onset of valley transfer and increases the mean steady state drift velocity v. For higher fields v is reduced, because the reduced cooling efficiency of the "hot" LO phonons leads to a higher Γ-valley temperature and therefore to a higher *population of* the L-valleys of lower mobility. Both the drag- and the heating-induced corrections amount to more than 20 percent at the highest investigated carrier concentrations (several 10^{17}/ccm).

In these calculations the integration of the time-dependent Boltzmann equation for the phonon distribution functions was performed in parallel to the number-, energy- and momentum balance for the *HDM* electrons in the Γ- and L-valleys for the momentary phonon distribution, implying an instantaneous adaption *of the carriers to any change* in the phonon population. However, besides the well-known HDM requirement of an extremely fast internal carrier thermalisation, such a complete enslavement of the carriers by the LO phonons would be justified only if the energy and momentum relaxation rates of the carrier system as a whole were much larger than the rate of change of the LO-phonon distribution. This condition is well fulfilled for the dominant polar optical electron–LO phonon coupling and was therefore sufficient for the investigation of the eventual approach to *a steady state and corresponding* stabilisation of the carrier-phonon system. But the model did not allow a detailed estimate of the initial transients and especially of the overshoot phenomenon, where the comparable time scales for the $\Gamma - L$ valley transfer and the LO-phonon buildup require a treatment of the time evolution of both carriers and phonons on the same footing.

So two questions remained:

(1C) Would a rapid initial phonon heating and the ensuing rise of the mean energy of the Γ-electrons *lead to an accelerated* $\Gamma - L$ transfer and thereby to a reduction of the overshoot through the earlier bend down of the mean carrier velocity.

(1D) Would this earlier onset of the transfer very soon reduce the number of fast-drifting Γ-electrons below its threshold value for strong LO-phonon amplification; in this case the phonon avalanche would be automatically quenched in its initial stages and the nonequilibrium-phonon effects kept low.

The present research project was set up to clarify these points within the model-free and highly effective Monte Carlo approach.

2. Scope and Objective of "Submicron Phononics II"

The scope of the project was

(2A) to implement nonequilibrium phonon *distributions into a conventional* Monte Carlo electron transport simulation.

The objectives of the project were:

(2B) to use the new code for a simulation of the simplified model of low- temperature steady-state acoustic phonon-electron transport in GaAs.

(2C) to extend this model to a fully time-dependent (transient) calculation of optical phonon interactions with near ballistic electrons in n-GaAs in the overshoot regime at room temperature (1) by modifying standard Monte Carlo codes to accommodate the numerical procedures required for nonequilibrium phonon calculations; (2) by applying these to real device phenomena such as picosecond response in n-GaAs to a *high field pulse*.

(2D) to collaborate with Professor Hess (University of Illinois) to ensure that the computer algorithms are included in his *Monte Carlo* codes.

3. Results

(3A) regarding item (2A):

In collaboration with M.Rieger (Univ.Graz) and with P.Bordone, C.Jacoboni, P.Lugli, and L.Reggiani from the University of Modena (Italy) a very general Monte Carlo code has been developed, which includes *a full Monte Carlo treatment of the phonon distribution* and provides the first model-independent transport theory of nonequilibrium carrier-phonon systems. The code provides for conventional one-particle simulation of steady-state transport as well as for ensemble simulation of time-dependent transport, displaying the important carrier parameters (such as densites, mean drift velocities and energies, and eventual changes of screening parameters), the scattering statistics of carriers and phonons, and the phonon distribution as *function* of the magnitude and orientation of the phonon wavevector. The program, of the conventional sequential type, is written in FORTRAN, and was run on the VAX 785 of the University of Graz (its general flow chart is shown below).

(3B) regarding item (2B):

Instead of the originally planned simulation of nonequilibrium electron - acoustic phonon systems in GaAs the more interesting case of low- temperature nonlinear transport of holes in p-Ge has been studied. Using the purely electronic one-particle Monte Carlo code of the Modena group, with analytical nonequilibrium phonon distributions (from "Submicron Phononics I") whose carrier parameters were obtained from the conventional carrier simulation in an iterative way, indications of a nonequilibrium - LA phonon-induced *current saturation* were found and confirmed by more complete HDM-model calculations (References 1 and 2 below).

(3C) regarding item (2C):

To test the full Phonon Monte Carlò, but to circumvent the very time-consuming anisotropic scattering *dynamics for the strongly peaked phonon distributions in high-d.c.field transport, the simpler case of isotropic* phonon amplification during the energy relaxation of laser-pulse excited carriers in GaAs was successfully simulated (References 3 and 5). The leading investigator in these studies was P.Lugli. These results confirmed earlier hot-carrier calculations of the Graz group, showing the decisive role of LO phonon amplification for the slowing down of the thermalisation of highly excited electron-hole plasmas (Reference 4).

Finally the main objective of the present project was achieved by the application of the code (3A) to the transient high-field response of n-GaAs. It confirmed the physical picture of the earlier DHM results (Sections 1A and 1B above) *about the effectiveness of the intervalley transfers to prevent the development* of a nonequilibrium-phonon induced instability and to ensure the approach to a steady state for fields of up to several ten kilovolts/ccm. Moreover, it was demonstrated that the initial LO-phonon amplification is also sufficiently quenched to prevent the destruction or reduction of the velocity overshoot, corroborating the hypothesis (1D) and thereby ruling out the hypothesis (1C) of our introductory discussion. These results *are summarised in Figures 1 to 5 below (from Reference 5)*

(3D) regarding item (2D):

The VAX compatibility of our code should guarantee a straightforward implementation of our program

on Professor Hess' CRAY system. We expect Professor Hess to arrange the necessary exchange of technical details and/or manpower to fulfil this last objective of the project.

4. Publications

1) P.Bordone, C.Jacoboni, P.Lugli, L.Reggiani, P.Kocevar: "Monte Carlo Analysis of Hot-Phonon Effects on Nonpolar Semiconductor Transport Properties", Proc.4th Int.Conf. on *Hot Electrons in Semiconductors*, Innsbruck 1985, Eds. G.Bauer, E.Gornik, and E. Vass, Physica 134 B, 169-173 (1985).

2) *P.Bordone, C.Jacoboni, P.Lugli, L.Reggiani, P.Kocevar: "Effect of a Perturbed Acoustic Phonon Distribution* on Hot Electron Transport: A Monte Carlo Analysis", J. Appl.Phys. 61, 1460-1648 (1987).

3) *P.Lugli, C.Jacoboni, L.Reggiani, P.Kocevar: "Monte Carlo Algorithm for Hot Phonons in Polar Semiconductors"*, Appl.Phys.Lett. 50, 1251-1254 (1987).

4) *P.Kocevar: "Hot Phonons", Festkörperprobleme (Advances in Solid State Physics) 27, 197-222 (1987).*

5) P.Lugli, C.Jacoboni, L.Reggiani, P.Kocevar: "Dynamical Simulation of a Perturbed Phonon Distribution *Induced by Hot-Carrier Thermalisation in GaAs", SPIE Proc. Vol.793 (1987)*: Conf.on Ultrafast Lasers Probe Phenomena in Bulk and Microstructure Semiconductors, Bay Point, U.S.A.,1987; to be publ.

6) M.Rieger, P.Kocevar, P.Bordone, P.Lugli, L.Reggiani: "Transient Hot- Phonon Effects on the Velocity Overshoot of GaAs: A Monte Carlo Analysis", Proc.5th Int.Conf.on Hot Carriers in Semiconductors, Boston, 1987; Ed.J. Shah; Solid State Electron.,to be publ.

5. List of Participating Personnel

P.Kocevar, Institut f. Theoretische Physik, Universitaet Graz, Austria
M.Rieger, Institut f. Theoretische Physik, Universitaet Graz, Austria

December 1987

(Dr.P.Kocevar)

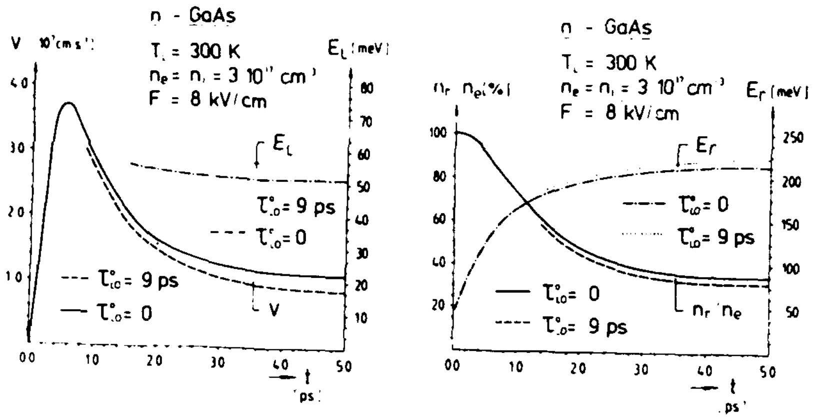


Fig.1: Time evolution of the mean carrier velocity v, the mean energies E_Γ and E_L of Γ- and L-valley electrons, and the relative Γ-valley population n_Γ/n_e. Full and dashed-dotted lines: phonon equilibrium ($\tau^0_{LO} = 0$); dashed and dotted lines: perturbed phonons; τ^0_{LO} is the $T_L \to 0$ limit of the LO-phonon thermalisation time τ_{LO}.

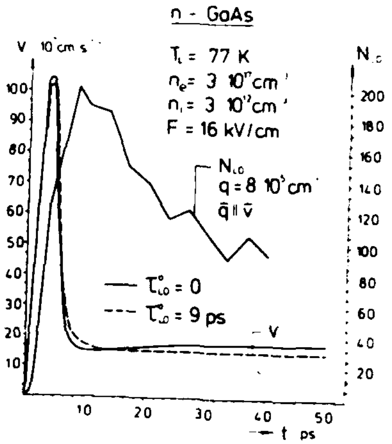


Fig.4: Velocity overshoot and amplification of a strongly coupling LO-phonon mode for the case of remote i-i scattering.

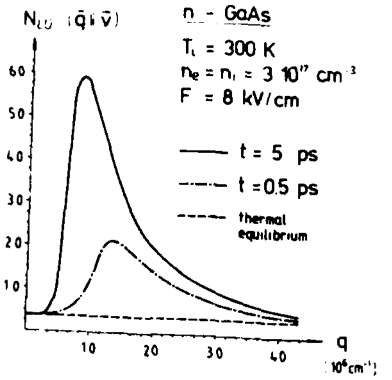


Fig.2: Time evolution of the LO-phonon distribution $N(\vec{q}, t)$ for forward modes ($\vec{q} \parallel \vec{v}$).

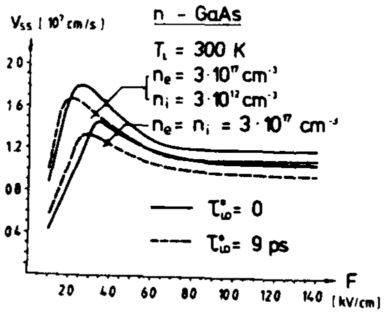


Fig.3: Steady-state velocity-field characteristics with and without phonon disturbances in the presence and absence of ionised-impurity scattering.

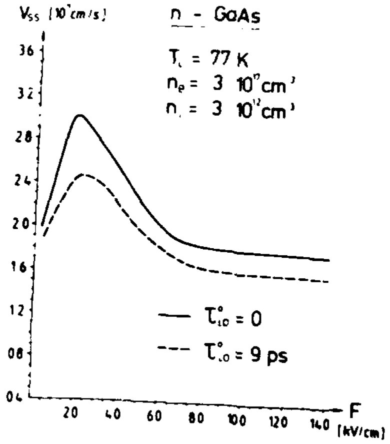
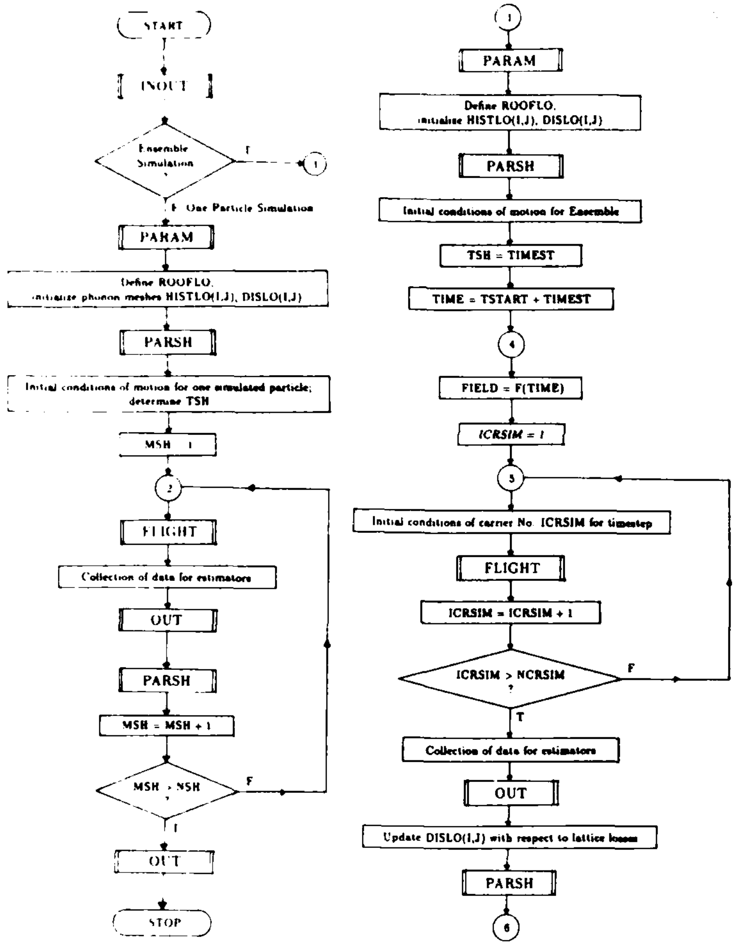


Fig.5: Steady-state velocity-field characteristics for the case of remote i-i scattering.

FLOW-CHART

MAIN PROGRAM



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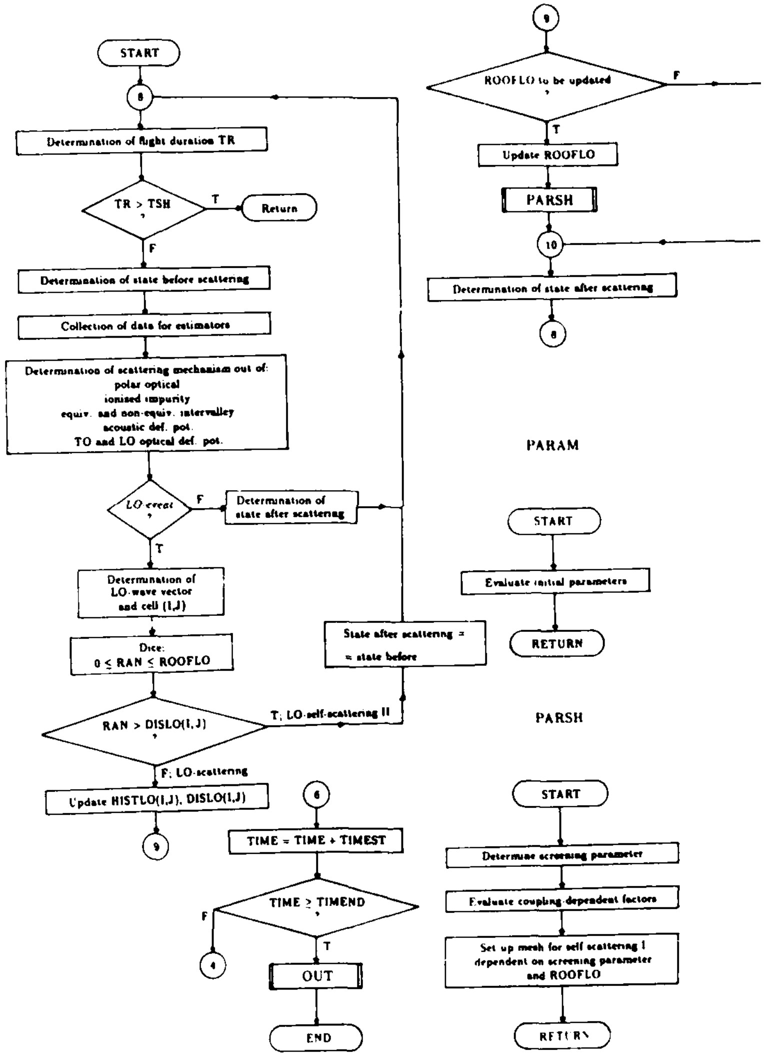

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