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MICROSCOPIC MODELS IN HOT ELECTRON PHENOMENA

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This paper reports on microscopic models which enable drift velocity, diffusion coefficient and white-noise temperature to be interpreted under hot-electron conditions. The analysis is devoted to covalent semiconductors diamond, Si and Ge.

1. Introduction

Taking advantage of the Monte Carlo technique [1], which provides an exact solution of the Boltzmann equation, this paper reports a systematic analysis of high-field phenomena in elemental semiconductors of group four. The main objective is to present a microscopic theory which for both types of carriers, holes and electrons, interprets three main aspects of transport phenomena, namely: drift, diffusion and white-noise. The band structure and scattering mechanisms characteristic of each material are the basis of such a theory.

2. Theory

A well accepted macroscopic definition of the drift velocity $\vec{v}_d$ and diffusion coefficient $\tilde{D}$ (*) can be given in terms of conductivity and diffusion current densities $\vec{j}_c$ and $\vec{j}_d$ by

$$\vec{j}_c = e\, n\, \vec{v}_d \tag{1}$$

$$\vec{j}_d = - e\, \tilde{D}\, \nabla n \tag{2}$$

n being the carrier concentration and e the algebraic charge of the carrier. Provided the two-terminal device made with the material of interest exhibits a positive value of real small signal impedance, Re(Z), and carrier-carrier scattering is neglected (**), the equivalent noise temperature associated with velocity fluctuations T_n can be related to the diffusion coefficient by the Shockley impedance field formula [6] through

$$T_n = \frac{e^2}{K_B\, Re(Z)} \int_\Omega n(\vec{r})\, \nabla z(\vec{r})\, \tilde{D}\left[\vec{E}(\vec{r})\right]\, \nabla z^*(\vec{r})\, d\Omega \tag{3}$$

(*) Possible generalizations concerning the definition of $\tilde{D}$ can be found in several papers [2,3] and in the lecture of J.P. Nougier in [4].

(**) A recent analysis of the effect of carrier-carrier scattering on fluctuation problems under non-equilibrium conditions can be found in [5].

Table 1 - Bulk constants of covalent semiconductors *

	diamond [13]	Si [14]	Ge [14]	units
ρ	3.51	2.33	5.32	gr/cm^3
u_l	$18.2\ 10^5$	$9.0\ 10^5$	$5.4\ 10^5$	cm/sec
u_t	$12.3\ 10^5$	$5.3\ 10^5$	$3.2\ 10^5$	cm/sec
θ_{op}	1938	735	430	K

* Notation: ρ is the crystal density, u_l and u_t are the longitudinal and transverse sound velocity, θ_{op} is the equivalent temperature of the long-wavelength optical phonon

Table 2 - Band parameters of holes *

	diamond	Si	Ge	units
$\|A\|$	3.61 [17]	4.22	13.38	-
$\|B\|$	0.18 [17]	0.78	8.48	-
$\|C\|$	3.76 [17]	4.80	13.14	-
Δ	0.006	0.044	0.295	eV
$m_h(\epsilon/\Delta \ll 1)$	0.53	0.53	0.346	-
$m_h(\epsilon/\Delta \gg 1)$	1.08	1.26	0.73	-
$m_l(\epsilon/\Delta \ll 1)$	0.19	0.155	0.042	-
$m_l(\epsilon/\Delta \gg 1)$	0.36	0.36	0.25	-
E_1^o	5.5	5.0	4.6	eV
d_o	61.2	26.6	40.3	eV

* Notation: A, B, C, are the inverse valence band parameters, Δ is the spin-orbit energy, ϵ is the hole energy, m_h, m_l are the density-of-states effective mass of heavy and light hole, E_1^o is an average acoustic deformation potential, d_o is the optical deformation potential. For references see the seminar of L. Reggiani [4]

K_B being the Boltzmann constant, $\vec{\nabla} z(\vec{r})$ the impedance field and the integration is performed on the volume of the device Ω. In analogy with $\tilde{D}$, T_n can be measured longitudinal and transverse to the direction of the current. The importance of eq.(3) results from the fact that in recent years it has provided the theoretical ground on which experimental information on $\tilde{D}$ has been obtained through noise-conductivity measurements by different European groups [7-11]. Conversely, as reported in the following, from a theoretical calculation of $\vec{v}_d$ and $\tilde{D}$ eq.(3) enables a microscopic interpretation of T_n to be carried out.

By using the moment method, the microscopic definition of $\vec{v}_d$ and $\tilde{D}$ which follows from eqs.(1,2) with the aid of the continuity equation [12] gives for an electric field along $\hat{x}$ direction:

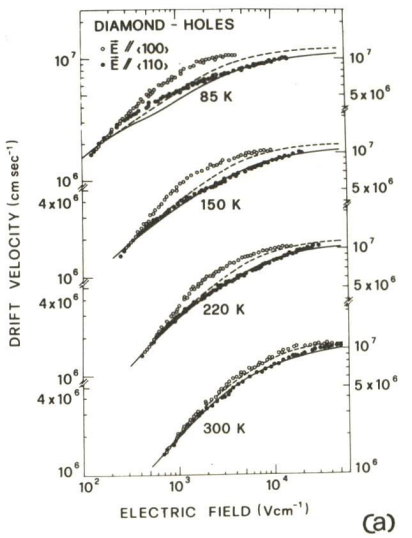
$$v_d = \frac{d}{dt}\langle x \rangle \qquad (4)$$

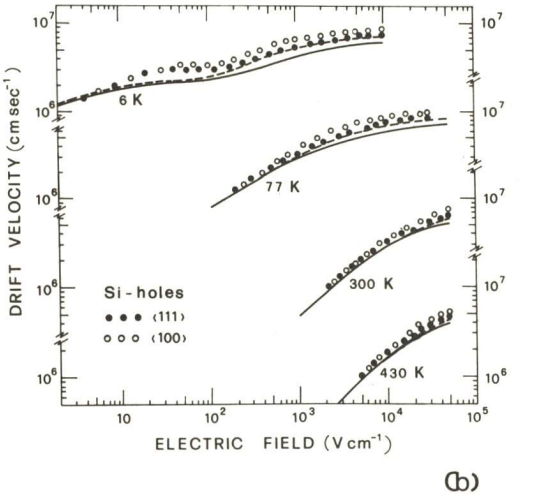
$$D_{xy} = \frac{1}{2}\frac{d}{dt}\left(\langle xy \rangle - \langle x \rangle \langle y \rangle\right) \qquad (5)$$

x and y being the distances covered along x and y directions by one carrier at a time t and $\langle\ \rangle$ indicating ensemble average. It should be noted that as time increases v_d and D, as defined from eqs.(4,5), tend to assume values which are independent of t. At very short times, the non-linear dependence of different moments on time will be of use to provide information on transient regime conditions.

3. Microscopic models, results and discussion

For most semiconductors energy band structure and phonon spectrum can be taken as temperature and electric field independent with good approximation. Therefore it is reasonable to expect the existence of microscopic models which are physically plausible and which enable an interpretation of hot-electron phenomena to be carried out within a wide range of electric field strengths and temperatures. Consequently, the simultaneous interpretation of drift, diffusion and white-noise within the same microscopic model can be assumed as a reliable test of both theoretical and experimental results. As a result, the case of covalent semiconductors, diamond, Si and Ge is analyzed when hot-electron phenomena are controlled by lattice





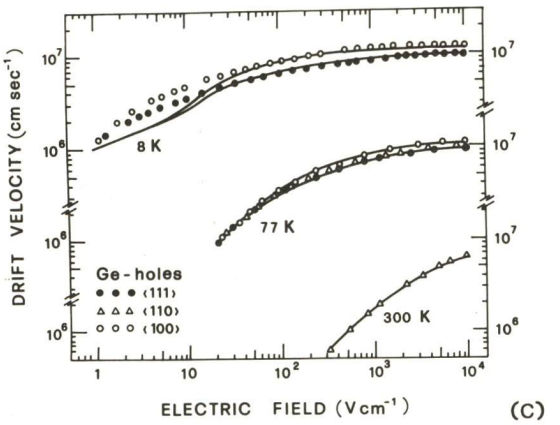


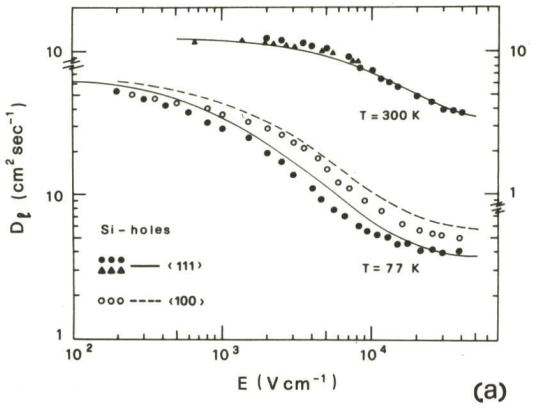
Fig. 1 - Drift velocity of holes as a function of electric field strength in (a) diamond [18], (b) Si [14] and (c) Ge [14]: Points present experimental data, lines report theoretical results

scattering only. The relevant abundance of recent experimental data together with the opportunity of reporting comparative and systematic results justify this choice. Table 1 reports the bulk constants used in calculations.

Holes

The band structure of holes in covalent semiconductors is very similar and a $\vec{k}\cdot\vec{p}$ analysis was found to describe well the energy wave-vector relationship [15]. Owing to its larger effective mass, heavy holes mostly determine electric field transport, consequently a one-band model which includes warping and non-parabolic effects in the way reported in [16] is used. Table 2 reports the values of the parameters used in calculations. A selected summary of available results on drift velocity, diffusion coefficient and white-noise temperature is reported for the materials cited in Figs.(1-4).

The anisotropy of v_d and D_l is found to be correlated to the warping of the heavy-hole band, larger values of both quantities arising for the direction along which the conductivity effective mass is smaller. At the lowest temperatures a



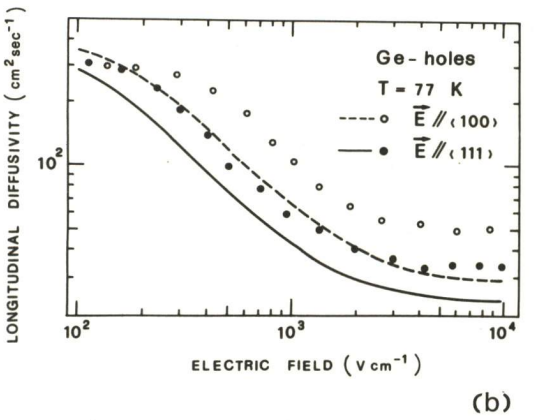


Fig. 2 - Longitudinal diffusion coefficient of holes as a function of electric field strength in (a) Si [19] and (b) Ge [14] : Open and closed circles present experimental data obtained with the time-of-flight technique, triangles with noise conductivity technique, the lines report theoretical results

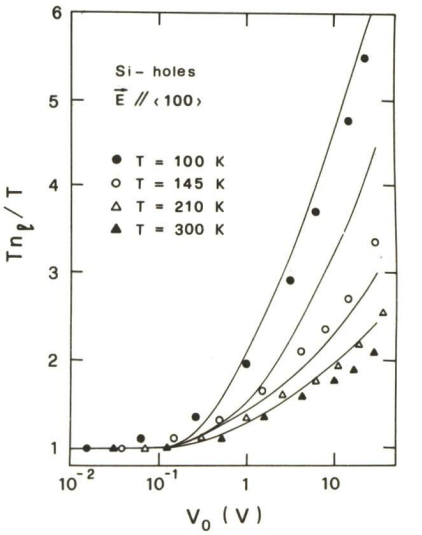


Fig. 3 - Normalized longitudinal noise temperature of holes in Si as a function of applied voltage in devices under space-charge-limited currents: Different points present experimental data [20] , the lines report theoretical results [21]

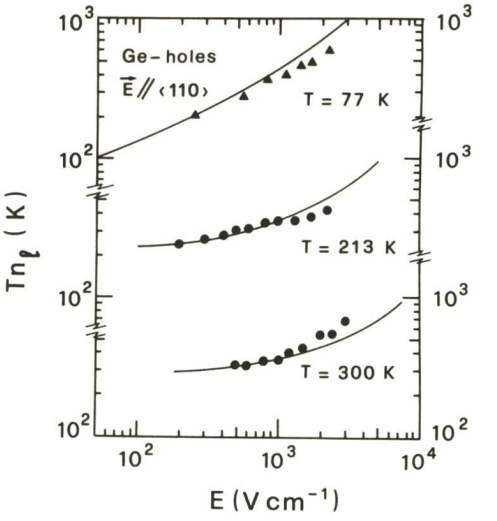


Fig. 4 - Longitudinal noise temperature of holes in Ge as a function of electric field strength: Triangles and full circles present experimental results [7,9], lines report theoretical results

saturated region of v_d and D_l is found at the highest electric field strengths. This effect is found to be correlated with the concomitance effect of both strong non-polar optical interaction and with non-parabolic behaviour of the energy wave-vector relationship. The dependence of T_n on electric field strength results from the concurrent

Table 3 - Band parameters of electrons *

	diamond	Si [14]	Ge [23]	units
ϵ_Δ	-	-	0.18	eV
ϵ_L	7.22 [17]	0.74	-	eV
ϵ_Γ	6.22 [17]	2.95	0.14	eV
$m_{l\Delta}$	1.4 [24]	0.98	1.35	-
$m_{t\Delta}$	0.36 [24]	0.19	0.29	-
m_{lL}	-	-	1.59	-
m_{tL}	-	-	0.08	-
m_Γ	-	-	0.04	-
$E_{1\Gamma}$	-	-	5	eV
E_{1L}	-	-	11	eV
$E_{1\Delta}$	8.7 [24]	9.5	9	eV
$(D_tK)_L$	-	-	5.5	10^8 eV/cm
Inter $\Delta\Delta$ θ_{g1}	1900 [24]	140	100	K
$(D_tK)_{g1}$	8 [24]	0.5	0.789	10^8 eV/cm
θ_{g2}	-	210	430	K
$(D_tK)_{g2}$	-	0.8	9.46	10^8 eV/cm
θ_{g3}	-	700	-	K
$(D_tK)_{g3}$	-	3	-	10^8 eV/cm
θ_{f1}	1560 [24]	210	-	K
$(D_tK)_{f1}$	8 [24]	0.15	-	10^8 eV/cm
θ_{f2}	1720 [24]	500	-	K
$(D_tK)_{f2}$	8 [24]	2.5	-	10^8 eV/cm
θ_{f3}	-	630	-	K
$(D_tK)_{f3}$	-	4	-	10^8 eV/cm
Inter$_{LL}$ θ_{LL1}	-	-	320	K
$(D_tK)_{LL1}$	-	-	3.0	10^8 eV/cm
θ_{LL2}	-	-	120	K
$(D_tK)_{LL2}$	-	-	0.2	10^8 eV/cm
Inter$_{L\Delta}$ $\theta_{L\Delta}$	-	-	320	K
$(D_tK)_{L\Delta}$	-	-	4.06	10^8 eV/cm
Inter$_{L\Gamma}$ $\theta_{L\Gamma}$	-	-	320	K
$(D_tK)_{L\Gamma}$	-	-	2.0	10^8 eV/cm
Inter$_{\Delta\Gamma}$ $\theta_{\Delta\Gamma}$	-	-	320	K
$(D_tK)_{\Delta\Gamma}$	-	-	10	10^8 eV/cm
α_Δ	-	0.5	-	eV^{-1}
α_L	-	-	0.3	eV^{-1}

*

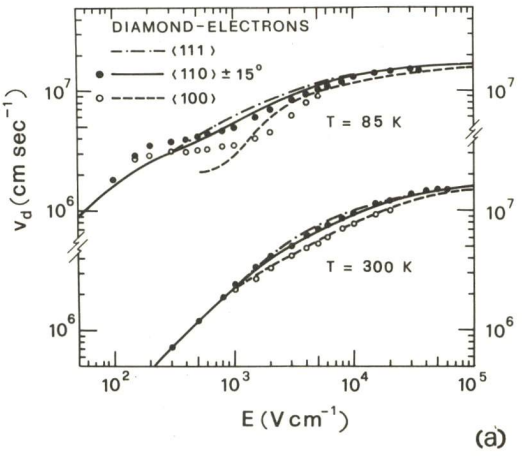
Notation: ϵ_Δ , ϵ_L, ϵ_Γ are the energy gaps measured from the conduction band minimum, $m_{l,t}$ are the effective masses, E_1 is the acoustic deformation potential, (D_tK) is the optical and/or intervalley coupling constant, θ is the equivalent temperature of the optical and/or intervalley phonon, α is the nonparabolic parameter

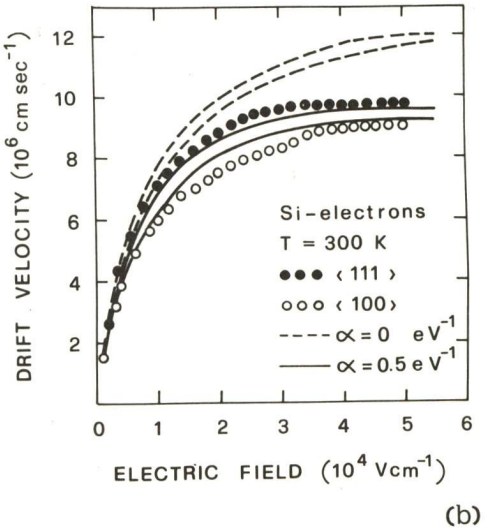
roles of drift and diffusion. The monotonic increase of T_n with applied voltage and electric field strength is correlated to the dominant role played by the sublinear behaviour of the drift velocity at increasing field strength.

Electrons

The band structure of electrons is similar for the case of diamond and Si. The same location of the conduction band minimum along Δ and the fact that higher minima at Γ and L points in the Brillouin zone are so high in energy as to be neglected justify the use of a single set of valleys which for the case of Si includes non-parabolicity effects in the way reported in [22] . For the case of Ge three sets of valleys with the minima at L which include non-parabolicity effects in the way reported in [23] should be used. Table 3 reports the values of the parameters used in calculations. A selected summary of available results on drift velocity, diffusion coefficient is reported for the materials cited in Figs.(5-7).

Anisotropy of v_d and D_l is correlated to the many-valley structure of the conduction band which, apart from a particular high-symmetry direction of the electric field ($\langle 111 \rangle$ in diamond and Si, $\langle 100 \rangle$ in Ge), leads different valleys to contribute in a different way to the total current and diffusion. So, anisotropy of v_d is well understood in terms of a repopulation of the different valleys. In fact, an increase of the population of the colder and slower valleys leads to reducing the total drift velocity with respect to the high symmetry direction. Anisotropy of D_l is related to an additional intervalley diffusion [27] which arises when electrons exhibit different





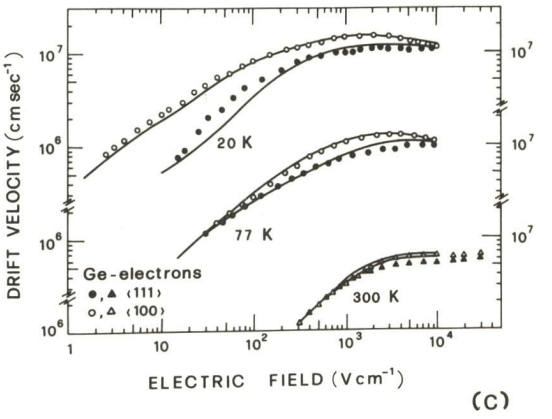


Fig. 5 - Drift velocity of electrons as a function of electric field strength in (a) diamond [24], (b) Si [14] and (c) Ge [14]: Points present experimental data, the lines report theoretical results

velocities in different valleys. This intervalley diffusion is found to give a valuable contribution to the total diffusivity which, in consequence, is enhanced with respect to the high-symmetry case.

Saturated regions of drift velocity are found at the highest field strengths for the case of diamond and Si. For the case of Si non-parabolicity has been found to play a valuable role. For the case of Ge at low temperatures ($T \lesssim 130$ K) and high fields a negative differential mobility (NDM) is present for $\vec{E}$ along ⟨100⟩ as well as ⟨111⟩ directions. It has been found that both non-parabolicity of the lowest minima and electron transfer to upper valleys give an effective contribution to the NDM phenomenon. No general conclusions have yet been reached on the behaviour of $\tilde{D}$ at the highest field strengths. As a result of non-parabolicity effect, theory does not predict a saturated region of D_1 which still needs experimental confirmation.

Transient regime

The study of the dependence on time of transport parameters at very short times combines with two basic interests: it promises further checks for existing microscopic models and hints at new physical phenomena. By briefly surveying this argument, two main lines of developments can be identified according to a semi-

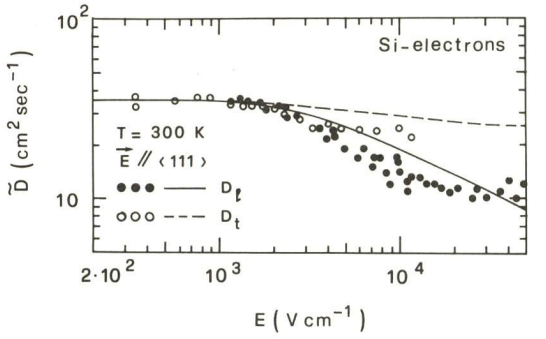


Fig. 6 - Diffusion coefficient of electrons in Si as a function of electric field strength: Open [25] and full [26] circles present experiments, lines report theoretical results

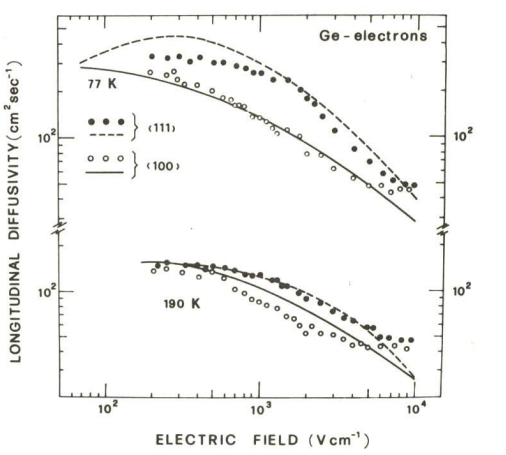


Fig. 7 - Longitudinal diffusion coefficient of electrons in Ge as a function of electric field strength: Open and full circles present experimental data, lines report theoretical results [14]

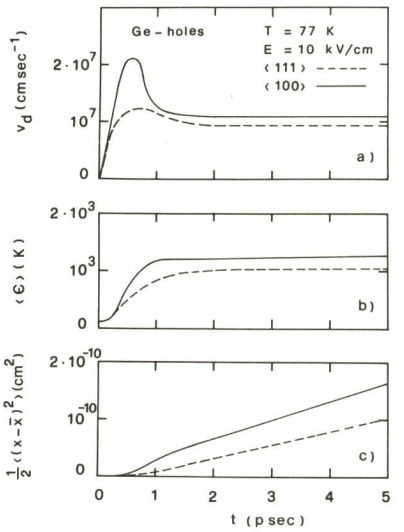


Fig. 8 - (a) drift velocity, (b) mean energy and (c) half mean-square displacement of holes in Ge as a function of time showing transient features

classical or quantum approach. The former approach considers the carrier collisions as occurring instantaneously in space and time, and investigates the behaviour of transport quantities such as drift, mean energy and diffusivity for times shorter than the stationary condition [28-30] . The main features of this phenomenon are the tendency of the drift velocity to exceed the stationary value for a brief period (velocity overshoot) and of the diffusivity not to follow Fick's law. Results of Monte Carlo calculations concerning transient regime of hot-holes in Ge at T = 77 K performed by making an ensemble average over 8192 simulations with an initial thermal distribution function assumed to be a Dirac one in space and energy and random momentum, are illustrated in Fig. (8). The latter approach attempts to account for the finite duration of the collision processes, thus investigating intra-collisional field effects (ICFE) [31-33] . The main features of ICFE, which both broaden and shift resonances, are to effectively lengthen the effective collision duration and weaken the effect of the collision itself. Supportive evidence of this phenomenon has been reported for the case of high-field transport in SiO_2 [34] .

4. Conclusions

Microscopic models which underlie the theoretical interpretation of drift, dif-

fusion and white-noise phenomena as function of electric field strength and temperature have been reported for the case of covalent semiconductors. Agreement between theory and experiments is somewhat better for drift velocity than for diffusion and white-noise temperature, discrepancies being confined within a factor two for these last quantities. The simplifications still existing in the model and the experimental uncertainty reasonably justify such a discrepancy. The most severe approximation still included in present models relies on the use of a simplified formulation for the deformation potential parameters which still forbid a "first principle" calculation of different quantities. New experimental data, as for example in the transient regime conditions, should motivate such a further improvement.

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