DYNAMIC SIMULATION OF THE ENERGY SPECTRUM
OF PHONONS IN THE MAGNETIC BCC IRON

Elena L. Angelova[#], Hassan Chamati

Received on October 1, 2021

Presented by Ch. Stoyanov, Corresponding Member of BAS, on November 30, 2021

Abstract

We used the symplectic and scalable algorithm for spin lattice dynamics embedded in LAMMPS to model the coupled relaxation processes of the spin and lattice subsystems to investigate the phonon dispersion of bcc Fe at $T = 300$ K. The atomic interactions were modelled via three semi-empirical many-body potentials within the embedded atom method, while the distance-dependent spin coupling relied on the Heisenberg-type Hamiltonian. In the state of mutual equilibrium of the spin and atom ensembles, we have calculated the dynamical matrix and the phonon spectra in bcc iron. We found that for a small to moderate wavevector absolute values, the phonon dispersion curves agree well with the experimental results obtained from inelastic neutron scattering, while discrepancies between theory and experiment were observed for larger wavevector values, particularly near the zone boundaries. Moreover, the impact of magnons on the phonon spectra is pronounced for all employed potentials.

Key words: computer modelling, interatomic potential, spin dynamics, bcc iron, spin-lattice coupling, phonon spectrum, magnons

[#]Corresponding author.

This work was supported by the European Regional Development Fund within the Operational Programme “Science and Education for Smart Growth 2014–2020” under the Project CoE “National Center of Mechatronics and Clean Technologies”, Contract No BG05M2OP001-1.001-0008.

DOI:10.7546/CRABS.2022.02.04

1. Introduction. Dynamic simulations of trajectories of atoms and molecules play a significant role in the study of collective phenomena in materials at finite temperatures. They became possible on a large scale thanks to the advancement of computing technologies and the development of powerful algorithms to perform molecular dynamics (MD) [1,2]. Being classical in nature, MD equations utilize different empirical or semi-empirical potentials with parameters depending on the contribution of the specific degrees of freedom of the material under consideration. Furthermore, the outcome of MD simulation depends on the environment, boundary conditions, symmetry, etc. To gain insights into materials at the nanoscale, along with the great possibilities of modern technology for manipulating the physical properties towards creating novel functional materials or modifying existing ones, MD simulations become an effective and powerful tool for nano-engineering [3]. To characterize the magnetic properties of materials, besides MD, spin-dynamics (SD) is proven to be an important tool for the investigations of materials with additional (spin) degree of freedom [4].

Spin dynamics equations may be integrated via MD [5]. This is achieved by combining the coordinate-dependent magnetic exchange interaction to a classical Hamiltonian with an atomistic potential. Using an empirical many-body potential and a parameterized exchange interaction in the frameworks of MD-SD, MA et al. [6] developed a dynamic simulation model for magnetic bcc iron where atoms are treated as classical particles with intrinsic spins. The analysis demonstrated the significant role played by spin degrees of freedom in the dynamics of motion of atoms in magnetic iron and iron-based alloys [6].

Over the years, the validity of the complex MD-SD approach and its applicability to the description of various thermodynamic processes has been confirmed in several papers [7–14]. Some authors [7–10] performed combined MD-SD simulations to investigate the mutual influence of phonons and magnons on their respective frequency spectra and lifetimes in ferromagnetic bcc iron. MUDRICK et al. [11] studied the dynamic properties of bcc iron with varying vacancy concentrations in MD-SD classical approach. MA et al. [12] employed MD-SD simulations to evaluate the difference between the free energies of bcc and fcc phases of magnetic iron, assessing their relative stability within a unified dynamic picture. In [13], the behaviour of the total energy and the norm of the total magnetization in fcc cobalt has been studied. PERERA et al. [14] proposed a powerful extension to MD-SD approach that fully captures the coupling between the atomic and spin subsystems via spin-orbit interactions. In [15] the magnetic behaviour of bcc iron nanoclusters was investigated by means of MD-SD, using a distance-dependent exchange interaction.

The goal of this paper is to advance our understanding of thermalization of the lattice and spin subsystems and excitations spectra in bcc ferromagnetic iron within the concept of MD-SD. We use three different embedded atom method (EAM) potentials [16–18] to describe the dynamic properties of bcc Fe at $T = 300$ K

with the aim to identify the potential that gives the most adequate explanation of both energy exchange between spin and lattice subsystems and quasiparticles spectra. In Section 2, we introduce the physical model and its parametrization, followed by a description of the computational methods we use for MD–SD simulations. Section 3 reports our results on both the thermalization of spin and lattice ensembles and the phonon spectra in bcc iron within MD–SD approach involving different potentials within the embedded atom method, followed by concluding remarks in Section 4.

2. Formalism. Recently, a symplectic and scalable algorithm for spin lattice dynamics was developed and embedded in the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [13]. Compared to classical molecular dynamics, this algorithm increases the phase space by assigning a classical spin vector $\mathbf{s}_i$ to each magnetic atom i at position $\mathbf{r}_i$, mass m_i and momentum $\mathbf{p}_i$. Then, for a system of N magnetic atoms the corresponding MD–SD Hamiltonian reads

$$(1) \quad H = \sum_{i=1}^N \frac{p_i^2}{2m_i} + \sum_{j,i \neq j}^N U(r_{ij}) - \sum_{i < j}^N J(r_{ij}) \mathbf{s}_i \cdot \mathbf{s}_j,$$

where the first term stands for the kinetic energy of iron atoms in the lattice, the second term $U(r_{ij})$ is the distance $r_{ij} = |\mathbf{r}_{ij}|$ dependent potential energy map, and the last term $J(r_{ij})$ is the magnetic coupling exchange energy, which emanates from two main contributions: (i) direct ferromagnetic exchange between the orbitals localized on the centres of ions i and j , and (ii) spin and charge polarizations effects provided by nonmagnetic orbitals. This MD–SD Hamiltonian possesses true dynamics, described by the following equations of motion of Fe atoms and their spins

$$(2a) \quad \frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m_i},$$

$$(2b) \quad \frac{d\mathbf{p}_i}{dt} = \sum_{j,i \neq j}^N \left[-\frac{dU(r_{ij})}{dr_{ij}} + \frac{dJ(r_{ij})}{dr_{ij}} \mathbf{s}_i \cdot \mathbf{s}_j \right] \mathbf{e}_{ij},$$

$$(2c) \quad \frac{d\mathbf{s}_i}{dt} = \mathbf{f}_i \times \mathbf{s}_i,$$

where $\mathbf{e}_{ij}$ is the unit vector along $\mathbf{r}_{ij}$, $\mathbf{f}_i$ is the analogue of a spin force applied on spin i . Mechanical interactions among atoms are computed using a many-body potential, and the interactions between spins are modelled with the Bethe–Slater curve

$$(3) \quad J(r_{ij}) = 4\alpha \left(\frac{r_{ij}}{\delta} \right)^2 \left(1 - \gamma \left(\frac{r_{ij}}{\delta} \right)^2 \right) e^{-\left(\frac{r_{ij}}{\delta} \right)^2} \Theta(R - r_{ij}),$$

where α , γ and δ are fitting parameters, based on the J values for bcc iron, $\Theta(R - r_{ij})$ is the Heaviside step function, and R is the cutoff radius.

The MD-SD is then determined via the set of coupled differential equations (2) for each atom i in the N atomic system under investigations. Hence, the total number of differential equations to be solved is $9N$.

It is worth mentioning that at equilibrium conditions, the instantaneous lattice temperature T_L is classically defined as a measure of the kinetic energy of the atoms

$$(4) \quad T_L = \frac{2}{3Nk_B} \sum_{i=1}^N \frac{p_i^2}{2m_i},$$

where k_B is the Boltzmann constant. On the other hand the spin temperature reads

$$(5) \quad T_S = \frac{\hbar}{2k_B} \frac{\sum_{i=1}^N |\mathbf{s}_i \times \mathbf{f}_i|^2}{\sum_{i=1}^N \mathbf{s}_i \cdot \mathbf{f}_i},$$

where $\hbar$ is the Planck constant. In [14], definition (5) has proven to be an efficient description of the thermalization of the spin subsystem and its relaxation toward thermal equilibrium during MD-SD simulations in bcc iron.

The phonon dispersion curves are computed with the aid of MD-SD methods. For the purpose of this study, we extend the approach proposed and implemented in LAMMPS in [19] to include spin dynamics. The details of our method will be published elsewhere.

3. Spin-lattice dynamics for Fe-bcc. 3.1. Initial conditions. The constructed triclinic box with periodic boundary conditions containing $8 \times 8 \times 8$ primitive cells (512 atoms) arranged in a bcc lattice is used in all equilibrium MD-SD simulations. For this box, size effects may be ignored since they do not affect the results. Starting from a lattice structure, for the ensemble of atoms the Gaussian initial velocity distribution is set with a mean of 0.0 and a mean squared deviation scaled to produce the temperature $T_L = 300$ K. The atoms were coupled by both the magnetic exchange interaction with coefficients from [13] and a real-space cutoff of 3.5 Å and one of the three mechanical EAM potentials, namely CHAMATI [16], CHIESA [17] and OLSSON [18] to describe the interaction among Fe atoms. These spin-less potentials are constructed without double-counting the ferromagnetic contribution to the mechanical energy. Both of the mechanical and magnetic potentials allow to reproduce known magneto-elastic properties in a correct manner [7,8,10,11,14,15]. The version of LAMMPS, dated 7Aug19, is used to investigate the physical properties of the coupled MD-SD in bcc Fe.

Initially, the orientation of the magnetic spin vectors of all Fe atoms was randomly distributed and the magnitude of each vector was set to the $2.2 \cdot \mu_B$. We allowed the atomic spin to move in time adiabatically according to a classical

model of Thomas's precession. Afterwards, we connected the system of magnetic spins associated to the atoms to a thermal bath. Moreover, we used a Langevin type thermostat for the spin subsystem and considered Brownian dynamics. Thus, the initial spin configuration corresponds to a magnetic equilibrium state at $T_S = 300$ K.

Starting from an initial lattice structure with zero linear momentum and highly paramagnetic spin state, the spin-lattice system was then equilibrated over 100 ps using the NVE symplectic time integration algorithm (with constant number of particles, volume and energy) with different values of the numeric integration timestep. Once the components of the spin vector were computed, both coordinates and momentum of atoms were updated via the Verlet method implemented in LAMMPS. During the run we computed both the temperature, the potential energy, the kinetic energy, the total system energy, and magnetic averaged quantities, such as the total magnetization of the system, the spin temperature, and the magnetic energy. These values were output every 50 timesteps over a total sampling time of 100 ps. Such time is long enough to obtain a convergent and size-independent MD-SD [13].

3.2. Phonon spectrum. To investigate the phonon spectra in bcc Fe at 300 K, first we perform a short microcanonical MD-SD equilibration run (typically about 20 000 time steps with $\Delta t = 5$ fs). This brings the whole system in the state of mutual equilibrium by resolving any inconsistency between the spin and atom ensembles. At the end of the run, both the lattice and the spin temperatures fluctuate about the mean value of the target temperature $T = 300$ K, showing that the lattice and the spin subsystems are in equilibrium. Then, we use the final output directly as the initial state for canonical ensemble simulations with fixed pressure and temperature. In this ensemble the equations of motion were integrated at 300 K with the same time step up to a total time of $t_{\max} = 32.5$ ns. The Nose-Hoover type thermostat and barostat were employed to maintain the system at 300 K and 1 atm. The elements of the dynamic matrix were printed out every 5000 measurements. Besides the dynamical matrix, throughout the entire trajectory, we printed the magnitude of the total magnetization, magnetic and lattice temperature, magnetic, kinetic, potential and total energy every 100 timesteps. As it is confirmed by the total energy and the total magnetization conservation in the time series, we reached a reasonable level of accuracy with the time step $\Delta t = 5$ fs. To obtain the phonon spectrum out of the dynamic matrices, we used the postprocessing code *phana* [19]. Figure 1 shows the phonon dispersion curves obtained from our MD-SD simulations corresponding to a temperature of 300 K in comparison to the experimental results obtained from inelastic neutron scattering [20]. For Chamati potential, the results for MD simulations without spin dynamics for the same temperature [16] are depicted too.

It is well known that the acoustic phonons spectrum in bcc iron consists of three branches. There are two transverse modes T_1 and T_2 which are degenerated

Fig. 1. Phonon dispersion curves obtained via MD-SD simulation (blue squares) and pure MD simulation (purple triangles) of a periodic block of bcc Fe atoms with the aid of Chamati [16] (top left), Chiesa [17] (top right) and Olsson [18] (bottom) EAM potentials. For comparison purposes, the experimental results obtained from inelastic neutron scattering [20] are also plotted with red dots

in common and one longitudinal mode L. Generally, the sound velocity for the longitudinal wave is higher than the one for the transverse wave. This condition is fulfilled for our spectra for phonons propagating in directions [100] and [110]. On the contrary, for the longitudinal acoustic waves propagating in the [111] direction phase velocity decreases near the zone boundary in respect to the phase velocity of the transverse wave. Moreover, for the longitudinal [111] acoustic waves we observe positive, negative and even zero group velocity.

It is seen that at 300 K, for all crystal directions, potentials employed ([16], [17] and [18]) and small to moderate wavevector absolute values q , both MD-SD and MD dispersion curves agree well with the results of the experiment. Difference between experimental data and calculation results is observed for larger q values, particularly near the zone boundaries. In the vicinity of the N point, along the [110] direction, for the transverse modes T_1 and T_2 the discrepancy is about 1.64 and 0.80 THz for the potential [16], respectively. For the other potentials from [17] and [18], these differences are 0.70 and 0.45 THz and 0.76 and 0.18 THz, respectively. A discrepancy between experimental and theoretical frequencies was also found for the longitudinal mode close to the H point for all EAM potentials

Fig. 2. The calculated by MD-SD fractional shift in transverse phonon frequencies in bcc Fe at $T = 300$ K in the lattice directions [100] (top left), [110] (top right) for T_1 mode, [110] (bottom left) for T_2 mode, and [111] (bottom right). Green, black and red squares correspond, respectively, to Chamati [16], Chiesa [17] and Olsson [18] EAM potentials

investigated, in absolute values 0.1, 0.39 and 0.22 THz for the potentials from [16], [17] and [18], respectively.

The discrepancies between theory and experiment can be explained by anharmonic effects not being faithfully captured in the three EAM potentials [16–18]. For Chamati potential, there is a deviation between MD-SD and MD phonon spectra for all q values, but it seems that the MD-SD approach describes the experiment better than MD alone (see Fig. 1). To examine the discrepancy between the MD-SD and MD phonon spectra for the employed potentials, we compare the characteristic frequencies determined from MD-SD simulations (ω_{MD-SD}) with the ones obtained from MD simulations (ω_{MD}) by calculating the fractional frequency shift $(\omega_{MD-SD} - \omega_{MD}) / \omega_{MD}$. The results are shown in Fig. 2, for the transverse mode, and in Fig. 3, for the longitudinal one. It is well seen that the phonon frequencies shift in the presence of magnons. This fractional shift up to 14% in absolute value is observed for all principal axes. A particularly interesting behaviour occurs for the transverse waves propagating in the [111] direction. Here we observed a dip in the curve calculated with use of Chiesa EAM potential [17] at $q \approx 0.6$. The bottom of the dip is close to zero. Therefore, the frequency of this phonon mode seems to be unaffected by the presence of magnons. On the contrary, for two other EAM potentials for the transverse waves propagating in

Fig. 3. The calculated by MD-SD fractional shift in longitudinal phonon frequencies in bcc Fe at $T = 300$ K in the lattice directions [100] (top left), [110] (top right) and [111] (bottom). Green, black and red squares correspond, respectively, to Chamati [16], Chiesa [17] and Olsson [18] EAM potentials

the same direction the fractional frequency shift does not vanish (see Fig. 2 bottom right). In [7], a similar dip in the dependence of the frequency fractional shift on the wavevector of the longitudinal phonon mode propagating in [111] lattice direction of bcc iron is found. Because the appearance of such dips strongly depends on the choice of the EAM potential, further experimental investigations are needed to explore the impact of the magnons on the phonon spectra in bcc iron.

4. Summary. In conclusion, we have successfully performed a serial implementation of coupled magnetic and molecular dynamics in bcc Fe at temperature $T = 300$ K. This is based on the SPIN package included in LAMMPS with symplectic Suzuki–Trotter decomposition of the spin propagation operators. The atoms were coupled by the magnetic exchange interaction and by one among the mechanical EAM potentials proposed in [16–18]. Langevin thermostats were applied to either the spin subsystem or the lattice subsystem.

The accuracy of the serial version of the coupled algorithm was analyzed in the microcanonical (NVE) statistical ensemble. Our goal was to verify that both the total energy of the Fe bcc system and the norm of the total magnetization were conserved along the 100 ps trajectories for all the EAM potentials employed. Using

the MD-SD simulations, we successfully reproduce the thermalization process of the spin and lattice subsystems. At the same time, the noticeable drift in the total energy values for all EAM potentials has been observed at timesteps ≥ 0.1 fs. As a whole, Chiesa potential proposed in [17] gives the smallest deviation of the total energy from its initial value. Further, at the investigations of phonons spectra in bcc Fe the dip in the dependence of the frequency fractional shift on the wavevector of the transverse phonon mode propagating in [111] lattice direction is potential-dependent. This behaviour is shown to be caused by the peculiarities of the models in which the electronic structure of the Fe atom is oversimplified and described in terms of empirical parameters. Although the EAM approach has the great merit of emphasizing the relevant mechanisms and rules, it cannot properly take into account the complex details of the electronic structure and is therefore unable to guarantee the fulfillment of the conservation laws. Overall, a rigorous parametrization of the potential could exclude the temporal fluctuations of the system energy. The application of this new potential will yield deeper insights into the thermal transport properties of the magnetic materials.

REFERENCES

- [1] RAPAPORT D. C. (2004) The Art of Molecular Dynamics Simulation, 2nd Edn, Cambridge, Cambridge University Press, [doi:10.1017/CB09780511816581](https://doi.org/10.1017/CB09780511816581).
- [2] FRENKEL D., B. SMIT (2002) Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, [doi:10.1016/B978-0-12-267351-1.X5000-7](https://doi.org/10.1016/B978-0-12-267351-1.X5000-7).
- [3] LAU D., W. JIAN, Z. YU, D. HUI (2018) Nano-engineering of construction materials using molecular dynamics simulations: Prospects and challenges, Composites Part B: Engineering, **143**, 282–291, [doi:10.1016/j.compositesb.2018.01.014](https://doi.org/10.1016/j.compositesb.2018.01.014).
- [4] LANDAU D. P., M. KRECH (1999) Spin dynamics simulations of classical ferro- and antiferromagnetic model systems: comparison with theory and experiment, J. Phys.: Condens. Matter, **11**, R179–R213, [doi:10.1088/0953-8984/11/18/201](https://doi.org/10.1088/0953-8984/11/18/201).
- [5] OMELYAN I. P., I. M. MRYGLOD, R. FOLK (2001) Algorithm for molecular dynamics simulations of spin liquids, Phys. Rev. Lett., **86**, 898–901, [doi:10.1103/PhysRevLett.86.898](https://doi.org/10.1103/PhysRevLett.86.898).
- [6] MA P. W., C. H. WOO, S. L. DUDAREV (2008) Large-scale simulation of the spin-lattice dynamics in ferromagnetic iron, Phys. Rev. B, **78**, 024434, 12 pp, [doi:10.1103/PhysRevB.78.024434](https://doi.org/10.1103/PhysRevB.78.024434).
- [7] PERERA D., D. M. NICHOLSON, M. EISENBACH, G. M. STOCKS, D. P. LANDAU (2017) Collective dynamics in atomistic models with coupled translational and spin degrees of freedom, Phys. Rev. B, **95**, 014431, 12 pp, [doi:10.1103/PhysRevB.95.014431](https://doi.org/10.1103/PhysRevB.95.014431).
- [8] PERERA D., D. P. LANDAU, D. M. NICHOLSON, G. M. STOCKS, M. EISENBACH et al. (2014) Phonon-magnon interactions in body centered cubic iron: A combined molecular and spin dynamics study, J. Appl. Phys., **115**, 17D124, [doi:10.1063/1.4863488](https://doi.org/10.1063/1.4863488).

- [⁹] PERERA D., D. P. LANDAU, D. M. NICHOLSON, G. M. STOCKS, M. EISENBACH et al. (2014) Combined molecular dynamics-spin dynamics simulations of bcc iron, J. Phys.: Conf. Ser., **487**, 012007, 9 pp, [doi:10.1088/1742-6596/487/1/012007](https://doi.org/10.1088/1742-6596/487/1/012007).
- [¹⁰] ZHOU Y., J. TRANCHIDA, Y. GE, J. MURTHY, T. S. FISHER (2020) Atomistic simulation of phonon and magnon thermal transport across the ferromagnetic-paramagnetic transition, Phys. Rev. B, **101**, 224303, 11 pp, [doi:10.1103/PhysRevB.101.224303](https://doi.org/10.1103/PhysRevB.101.224303).
- [¹¹] MUDRICK M., M. EISENBACH, D. PERERA, G. M. STOCKS, D. P. LANDAU (2017) Combined molecular and spin dynamics simulation of bcc iron with lattice vacancies, J. Phys.: Conf. Ser., **921**, 012007, 5 pp, [doi:10.1088/1742-6596/921/1/012007](https://doi.org/10.1088/1742-6596/921/1/012007).
- [¹²] MA P. W., S. L. DUDAREV, J. S. WROBEL (2017) Dynamic simulation of structural phase transitions in magnetic iron, Phys. Rev. B, **96**, 094418, 17 pp, [doi:10.1103/PhysRevB.96.094418](https://doi.org/10.1103/PhysRevB.96.094418).
- [¹³] TRANCHIDA J., S. J. PLIMPTON, P. THIBAudeau, A. P. THOMPSON (2018) Massively parallel symplectic algorithm for coupled magnetic spin dynamics and molecular dynamics, J. Computat. Phys., **372**, 406–425, [doi:10.1016/j.jcp.2018.06.042](https://doi.org/10.1016/j.jcp.2018.06.042).
- [¹⁴] PERERA D., M. EISENBACH, D. M. NICHOLSON, G. M. STOCKS, D. P. LANDAU (2016) Reinventing atomistic magnetic simulations with spin-orbit coupling, Phys. Rev. B, **93**, 060402(R), 5 pp, [doi:10.1103/PhysRevB.93.060402](https://doi.org/10.1103/PhysRevB.93.060402).
- [¹⁵] DOS SANTOS G., R. APARICIO, D. LINARES, E. N. MIRANDA, J. TRANCHIDA et al. (2020) Size and temperature dependent magnetization of iron nanoclusters, Phys. Rev. B, **102**, 184426, 15 pp, [arXiv:2007.02230](https://arxiv.org/abs/2007.02230), [doi:10.1103/PhysRevB.102.184426](https://doi.org/10.1103/PhysRevB.102.184426).
- [¹⁶] CHAMATI H., N. PAPANICOLAOU, Y. MISHIN, D. PAPACONSTANTOPOULOS (2006) Embedded-atom potential for Fe and its application to self-diffusion on Fe(100), Surf. Sci., **600**, 1793–1803, [doi:10.1016/j.susc.2006.02.010](https://doi.org/10.1016/j.susc.2006.02.010).
- [¹⁷] CHIESA S., P. M. DERLET, S. L. DUDAREV, H. V. SWYGENHOVEN (2011) Optimization of the magnetic potential for α -Fe, J. Phys.: Condens. Matt., **23**, 206001, [doi:10.1088/0953-8984/23/20/206001](https://doi.org/10.1088/0953-8984/23/20/206001).
- [¹⁸] OLSSON P. A. T. (2009) Semi-empirical atomistic study of point defect properties in BCC transition metals, Computat. Mater. Sci., **47**, 135–145, [doi:10.1016/j.commatsci.2009.06.025](https://doi.org/10.1016/j.commatsci.2009.06.025).
- [¹⁹] KONG L. T. (2011) Phonon dispersion measured directly from molecular dynamics simulations, Comp. Phys. Commun., **182**, 2201–2207, [doi:10.1016/j.cpc.2011.04.019](https://doi.org/10.1016/j.cpc.2011.04.019).
- [²⁰] MINKIEWICZ V. J., G. SHIRANE, R. NATHANS (1967) Phonon dispersion relation for iron, Phys. Rev., **162**, 528–531, [doi:10.1103/PhysRev.162.528](https://doi.org/10.1103/PhysRev.162.528).

Institute of Solid State Physics
Bulgarian Academy of Sciences
72 Tsarigradsko Chaussée Blvd
1784 Sofia, Bulgaria
 e-mails: angelova@issp.bas.bg
 chamati@issp.bas.bg