MODEL-INDEPENDENT EVALUATION OF RECOILS CHANNELING IMPACT ON VISIBLE ENERGY SPECTRA IN DARK MATTER PARTICLES CRYSTALLINE DETECTORS

S. V. Dyuldya, M. I. Bratchenko

National Scientific Centre “Kharkiv Institute of Physics and Technology”, Kharkiv, Ukraine

Proposed is a direct method of Dark Matter crystalline scintillation detectors calibration by means of an atomistic molecular dynamics modeling of their responses to ~10 keV recoil atoms. Simulations show that the recoils channeling exists in NaI lattice with probabilities of ~5 - 15 %. It does not affect the mean values of quenching factors but gives rise to high visible energy spectral tails absent in disordered detectors. As a result, the lattice ordering manifests the ~100 % effect on NaI(Tl) visible energy spectra at 2÷6 keV window.

Channeling [1, 2] is widely discussed in the Dark Matter (DM) community concerning its impact on interpretation of low-background DM direct detection with scintillation counters. The standard weakly interacting massive particles (WIMP) scenario of DM particles (DMp) assumes the detector light response to be only due to primary knock-on atoms (PKA) recoiled at DMp-nucleon elastic scattering. The PKA energies E_R range in $\sim 10^{(0\div 2)}$ keV at WIMP masses $M \sim 10^{0\div 2}$ GeV/c^2. A part $\Delta E_{el} = q_{el} \cdot E_R$ of E_R is transferred to electrons of a detector via ionization energy losses of the PKA induced atomic collision cascade. But the detected (*visible*) energy $E_{det} = q \cdot \Delta E_{el}$ is only a fraction $Q(E_R) = q_{el}(E_R) \times \times q(E_R)$ of E_R due to detector and PKA type specific quenching $q < 1$ of electronic excitations [3, 4]. Since one can identify E_R of a monoenergetic PKA source using the instrument probability distribution function (p.d.f.) $p_{det}(E_{det}|E_R) = \delta(E_{det} - Q \cdot E_R)$, proper quenching factors $Q(E_R) < 1$ are of key importance for reliable calibration of DMp scintillation detectors.

Channeling has been first introduced into this agenda by Drobyshevski’s [5] hypothesis that certain fraction $P_{ch} < 1$ of the recoils are channeled in a crystalline detector, and have abnormally high quenching factors $Q_{ch} = 1$. Thus actually $p_{det}(E_{det}|E_R) = P_{ch} \cdot \delta(E_{det} - E_R) + (1 - P_{ch}) \cdot \delta(E_{det} - Q \cdot E_R)$. The P_{ch} estimation model of DAMA collaboration [6] has predicted an enhancement of NaI(Tl) crystal counting efficiency in the near-threshold 2÷6 keV window of their 8σ significant observation of DM attributed annual modulation signal. They evaluated $P_{ch}(E_R)$ by means of the Monte Carlo (MC) procedure of ray-tracing of a point isotropic source of recoils, and qualified the channeled ones as those directed within the Lindhard critical angles $\psi_c(E_R)$ [1] of open axial and planar channels of NaI(Tl) single crystal. It resulted in a very significant ($P_{ch} \sim 25$ % for 4 keV I) channeling.

But the foundations of Refs. 5 and 6 look very questionable. An ansatz $Q_{ch} = 1$ [5] is definitely violated at keV energies since the elastic (nuclear) energy loss ΔE_n of well channeled heavy ions is non-negligible. The ΔE_{el} dominance at channeling was suggested in early 1960’s to predict [7, 8] its impact on a number $\nu(E_R)$ of atomic displacements in neutrons induced collision cascades in metals. But all attempts to observe the $\nu(E_R)$ reduction have lost out. The collaboration model [6] also omitted the blocking effect [1] of PKA strong scattering by the nearest neighbors of the lattice site of emergence. It has been critically revised in a semi-analytical model of Bozorgnia - Gelmini - Gondolo (BGG) group [9, 10] that suggested that the PKA capture into a channel requires its initial transversal thermal displacement beyond the critical distance $r_c(E_R) \sim 0.1 \div 1$ Å of stable channeling. Such a model has been first introduced by Kumakhov [8] in 1972, and similarly to his estimates for metals, the BGG model calculations for various detector materials result in exponentially small $P_{ch} < 1$ %.

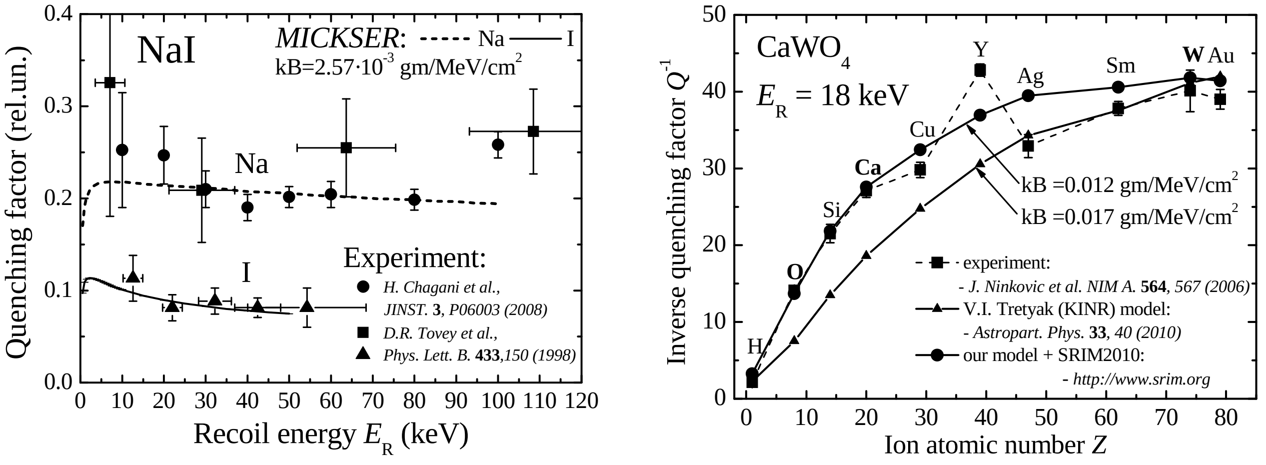
One can see that the situation remains far from clear since the results of application of different models differ by orders of magnitude. The essentially quantitative problem of DM detector calibration conflicts with the mostly qualitative nature of the low energy channeling analytical criteria. Besides, channeling is highly unstable due to intrinsic dechanneling on thermal vibrations and electrons, and is known to interfere with other competitive directional effect of crystal lattice ordering.

In the present work, we perform the channeling/blocking models independent atomistic simulation of the impact of NaI lattice ordering on detector readings. We compare responses in a crystalline and entirely disordered (amorphized) representations of the same detector material at preservation of all other simulation parameters. Our approach is free of *a priory* introduction of channeling that emerges by oneself in lattices. However, the *a posteriori* statistical analysis of collision cascade dynamics allows us to clarify its role and to suggest proper values of P_{ch} and Q_{ch}.

We use the in-house developed molecular dynamics (MD) code *MICKSER* [11]. It implements the restricted version of MD valid for simulation of atomic collisions in crystals and amorphous materials down to ~1 eV with special attention paid to accurate modeling of ion implantation, channeling, and other directional effects. Algorithmic details can be found in Ref. 11. Current version of the code is capable to model the full collision cascade by trajectory tracking of all atoms recoiled with energies exceeding the lattice binding energy $E_b < 10$ eV. The “universal” Ziegler - Biersack - Littmark (ZBL) interatomic potential was used in combination with the inhomogeneous electron densities calculated within the Isolated Atomic Density Superposition (IADS) method. Ionization stopping was calculated according the well-established Firsov and Brandt - Kitagawa models. The statistics of MC sampling of collision cascades was $\sim 10^4$ for each PKA energy E_R. The energies ΔE_n and ΔE_{el} deposited in a cascade into the nuclear and electronic subsystems of

NaI were tallied, while the cascade total energy $E_R = \Delta E_n + \Delta E_{el}$ was monitored to conserve within 0.1 % of E_R.

To calculate visible energies $E_{det} = q \cdot \Delta E_{el}$, applied is the novel modification of the classical Birks formula $q = (1 + kB \cdot |dE/dx|)^{-1}$ [3] with an empirically adjustable Birks constant *kB*. Instead, we use $q(E_R) = [1 + kB \cdot \Delta E_{el}(E_R)/R(E_R)|]^{-1}$ where ΔE_{el} is the total inelastic energy deposition in the PKA induced collision cascade and *R* is the PKA total range. It is based on the fact that the size of the coherent light response formation domain (~$10^{1 \div 3}$ nm) considerably exceeds the size of ~keV energy cascades (~*R*). The quantities $\Delta E_{el}(E_R)$ and $R(E_R)$ are readily computable by our *MICKSER* code as well as by the *SRIM* code, www.srim.org. It allows direct modeling of $Q(E_R)$, see Fig. 1 for this method validation. But further to *SRIM*, our code can also tally $q(E_R)$ as a random variate on a per-event (per-cascade) basis to make it possible the MC tallying of the visible energy E_{det} spectra.



a *b*

Fig. 1. The *MICKSER* and *SRIM2010* calculated quenching factors *Q* for various ions in disordered NaI (*a*) and $CaWO_4$ (*b*) compared to the experimental data and the results of Tretyak model calculations [4].

We start from the clear evidence of directional effects (incl. channeling) at recoil dynamics in NaI crystal lattice of NaCl type, lattice unit (l.u.) 6.473 Å. In Fig. 2, all ion flux angular maps are highly anisotropic, and correlated with NaI crystallography. Blocking dominates at 1÷2 l.u. from the PKA start point while at large distances *r* it gives place to relatively stable channeling. The momentum isotropization (that forms the uniformly grey maps in disordered NaI) is never reached here: due to energy losses only well channeled ions can be delivered to distances exceeding their range in the amorphized NaI. A similar dynamics appears for all other $E_R \subset (1 \div 100)$ keV. It means that the lattice driven anisotropy is characteristic for collision cascades under consideration.

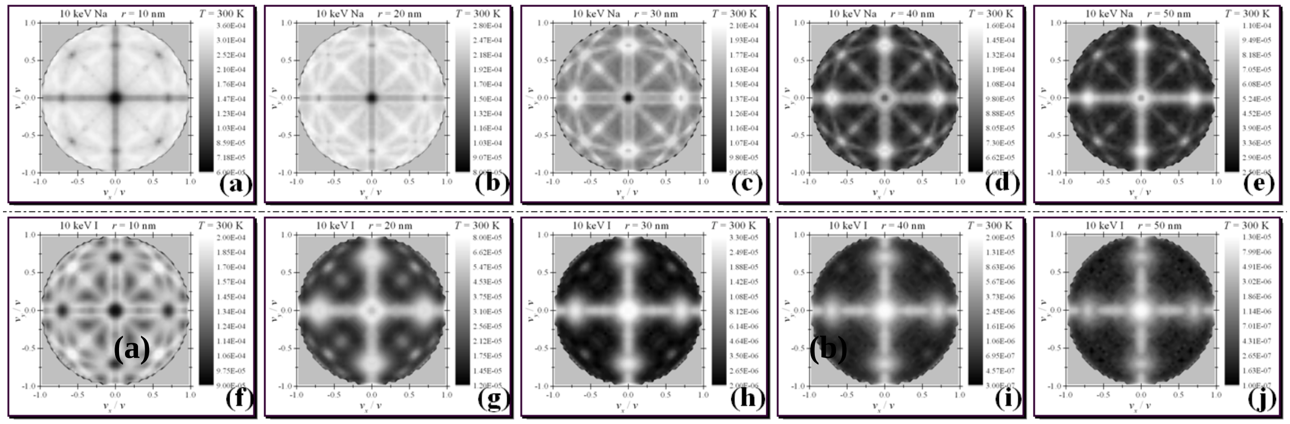
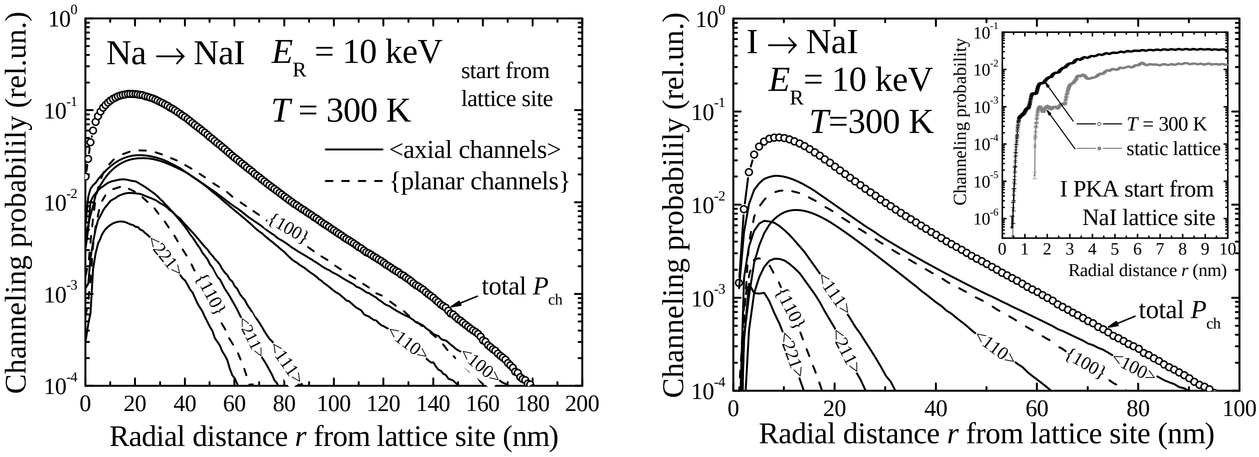


Fig. 2. Radial projections of total angular distributions of 10 keV Na (a→e) and I (f→j) PKA plotted at increasing distances $r = 10, 20, \rightarrow, 50$ nm from the NaI lattice site of their isotropic emergence at 300 K. Dark spots at small *r* correspond to blocking while light spots and strips indicate axial and planar channeling.

The *MICKSER* code capability of channeling identification (see details in Ref. 11) have enabled its quantitative rating by means of routine calculation of transversal energies $E_\perp$ in several dozens of channels and their comparison with theory supplied critical values. Fig. 3 presents the probabilities $P_{ch}(r)$ to find a recoil channeled at a distance *r* from the lattice site of its emergence.

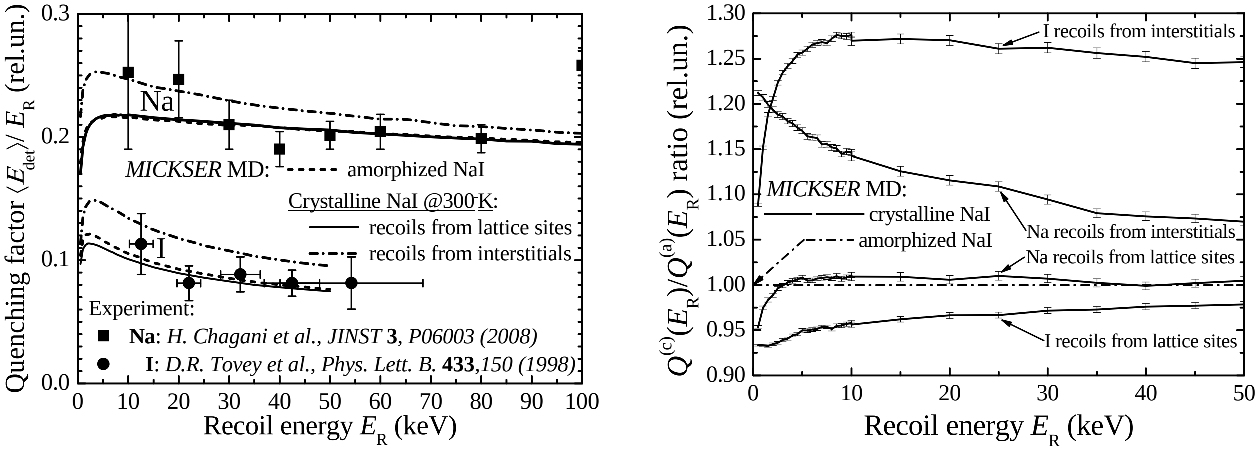


a *b*

Fig. 3. Radial dechanneling functions $P_{ch}(r)$ of 10 keV Na (*a*) and I (*b*) isotropically emerged recoils together with partial $P_{ch}(r)$ of the most significant axial <*hkl*> and planar {*hkl*} channels.

Evidently, and opposite to model assumptions of [5, 6, 9], $P_{ch} \neq$ const but is a “dechanneling function” of *r*. Due to blocking, P_{ch} is marginal (<0.1 %) at $r \leq (1\div2)\cdot$l.u. from a site. It agrees well with the analytical results of BGG group [9] and those of Kumakhov [8]. But a rapid volume capture [2, 11] into the channeling mode of recoil motion takes place at greater distances. It populates P_{ch} maxima to ≈15 % (Na) and ≈5 % (I) at $r \sim (10\div20)\cdot$l.u. Then $P_{ch}(r)$ decays exponentially. The inset of Fig. 3, *b* indicates that the capture is not exclusively owned [8, 9] to thermal displacements of the PKA start point. It occurs also in a regular static lattice at multiple small-angle scattering of recoils. We summarize the Fig. 3 data with the conclusion that the attempts [8, 9] to describe the recoil channeling probability P_{ch} by whatever local measure of its emergence initial conditions are insufficient. Channeling is populated non-locally in the bulk up to several percents high probability.

But does it affect the quenching factors of NaI(Tl) detectors? Fig. 4 argues that the answer is (most likely) negative. The lattice effect is significant (~10÷25 %) for PKA emergence from interstitial locations but is much smaller (~1÷5 %) for actual emergence from lattice sites. This is a challengingly small difference to be resolved experimentally, see Fig. 4, *a*. Fig. 4, *b* shows that Q_I in a crystalline NaI is ≈5 % smaller then in the disordered one. This effect cannot be due to channeling.



a *b*

Fig. 4. Quenching factors $Q(E_R)$ for Na and I induced cascades in crystalline$^{(c)}$ and amorphized$^{(a)}$ NaI (*a*) and comparative measure $Q^{(c)}/Q^{(a)}$ of lattice impact for different conditions of PKA emergence (*b*).

The weakness of $Q = \langle E_{det} \rangle / E_R$ lattice ordering sensitivity agrees with Lindhard’s reversibility rule [1, 2] that predicts the *in toto* compensation of channeling and blocking impacts on all mean (integral) yields of isotropic recoils’ atomic collisions (as noted above, the same is valid for $\nu(E_R)$).

However, this rule does not impose constraints on differential statistical distributions (p.d.f.) of measurable quantities. Fig. 5 shows that they are different in lattices and in disordered media. Unlike the Gaussian shaped spectra in amorphized NaI, both ΔE_{el} and E_{det} in a crystal manifest (i) exponential high-energy tails more pronounced for interstitial emergence and (ii) certain increase of probability of low-energy loss and E_{det}. The former feature is well attachable to channeling since it is statistically similar to the “channeling tails” of ion ranges, a known issue of ion implantation [11]. The less obvious root of the latter one is quasichanneling [12] at focusing of recoils onto atomic

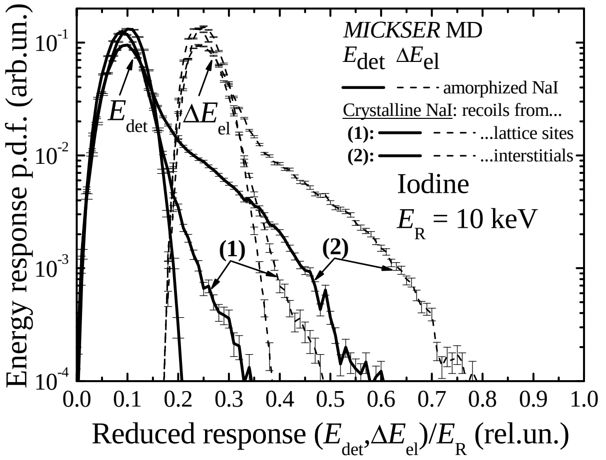
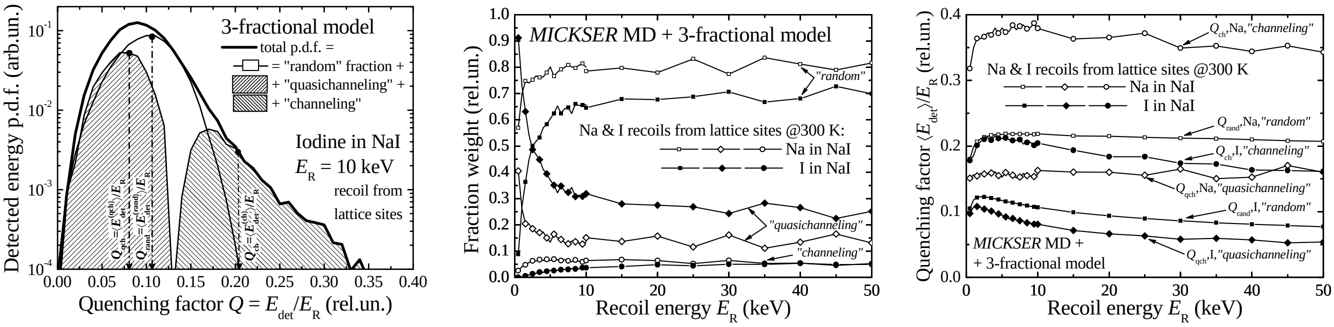


Fig. 5. Differential spectra of ionization energy losses and quenched visible energies for 10 keV cascade at different conditions of Iodine PKA emergence.

rows/planes. Quasichanneled ions experience a large nuclear energy loss that is localized at $r \leq (3 \div 5) \cdot$l.u. and thus renormalizes (softens) the energy available to the subsequent part of cascade. It is also responsible for the reduced Q of heavy Iodine in Fig. 4.

For Na PKA, the Fig. 5 spectra shift to the right and broaden. The same spectral shape is observed at all relevant PKA energies E_R. So, these lattice effects are common for crystal detectors. They can be qualified quantitatively by means of the Fig. 6, *a* 3-fractional fit representing the E_{det} p.d.f. $f\left(E_{det}\right) = \sum_{j=1}^{3} P_j f_j \left(E_{det}\right)$ as a P_j-weighted sum of partial p.d.f. f_j of random chaotic (*rand*), channeled (*ch*) and quasichanneled (*qch*) fractions of cascade dynamics, and making the only assumption that the $f_{rand}(E_{det})$ shape is the same one that is modeled in an amorphized version of NaI.



a *b* *c*

Fig. 6. 3-fractional model partitioned p.d.f. of Q (*a*); populations P_j (*b*); partial Q_j (*c*) of fractions.

One can see in Fig. 6, *b* that $P_{ch} \sim (3 \div 7)$ % for both Na and I PKA in a broad range of E_R. By order of magnitude, it agrees with the Fig. 3 data obtained using just another trajectory point dependent channeling criterion. The total population $P_{ch}+P_{qch}$ of lattice driven directional effects is ~20÷30 %. It is greater for Iodine due to more pronounced quasicahnneling of a heavier recoil. The first moments $\langle E_{det}\rangle_j = \int dE_{det} E_{det} f_j(E_{det})$ define the fractional quenching factors $Q_j = \langle E_{det}\rangle_j / E_R$ plotted in Fig. 6, *c*. The basic model assumption $Q_{ch} = 1$ of Refs. 5, 6, 9 definitely fails: though $Q_{ch} \sim 2 \cdot Q_{rand}$, all $Q_{ch} < 40$ %. The representative Q_{ch} are ≈0.35 (Na) and ≈0.2 (I). It is also notable that $Q_{qch} < Q_{rand}$.

We note that the simulated E_{det} spectra and the obtained "effective" (P_{ch},Q_{ch}) values differ substantially from those used in current treatments of the channeling impact. So, it is of great interest to examine how they affect the visible energy spectrum in the DAMA detector. It can be studied using the standard approach of the Lewin-Smith compendium [13] but applying the MD simulated p.d.f. $f(E_{det}|E_R)$ instead of conventional δ-shaped $p_{det}(E_{det}|E_R)$. We have carried out a pilot evaluation using the PKA energy spectra dR/dE_R for spin-independent WIMP-nucleon elastic scattering with total $\sigma_0 = 10^{-6}$ pb and Helm form factor. The Ref. [13] galactic halo model was used: the Earth velocity annual span $v_E = 244 \pm 15$ km/s, the DMp escape velocity $v_{esc} = 600$ km/s, the near-earth DM mass density $\rho_{DM} = 0.74\,\mathrm{GeV \cdot c^{-2} \cdot cm^{-3}}$. For NaI, the composite $dR(E_R)/dE_R$ is upper bounded by the kinematical maximal energy transfer $E_R^{(max)}$ of Na (≈80 keV at WIMP mass 20 GeV/c^2), and decays *abt* exponentially with an inflection at $E_R^{(max)} \approx 40$ keV of I. The properly interpolatable database of pre-modeled $f(E_{det}|E_R)$ for $E_R \subset 10^{(0 \div 2)}$ keV was used in calculations. The results are shown in Fig. 7.

In Fig. 7, *a*, DAMA model [6] shows the ubiquitous impact of channeling. According to BGG model [9], it appears only above the quenched limit $E_{det}^{(max)} = Q_{Na} \cdot E_R^{(max)} = 24$ keV. The MD based data of Fig. 7, *b* - *d* manifest just an intermediate case: the relative magnitude of lattice driven effects is ~100 % at 2÷6 keV visible energies (*cf.* ~1000 % of DAMA and ~1 % of BGG models; note that our results tend to DAMA ones for unrealistic interstitial emergence). The lattice effect in these bins is due to Iodine recoils. In Fig. 7, *c*, its amplitude grows *abt* linearly with WIMP mass while shifting to higher E_{det} and thus leaving the window of the collaboration observed DMp signature.

The reason of the obtained lattice ordering provided increase of detector response consists in the existence of channeling tails of Fig. 5. Owing to them, the recoils of lower E_R can contribute to the specific bin of visible energy E_{det}. Recently, such tails have been also observed, and correlated to anomalously high recoil ranges, by the South Korean group [14] at their simulations of CsI(Tl) detector. The *MARLOWE* code simulated [14] tail in CsI crystal for E_R = 18.4 keV is populated to ≈4.5 % fairly consistently with our MD evaluation of Fig. 6, *b* for NaI crystalline detector.

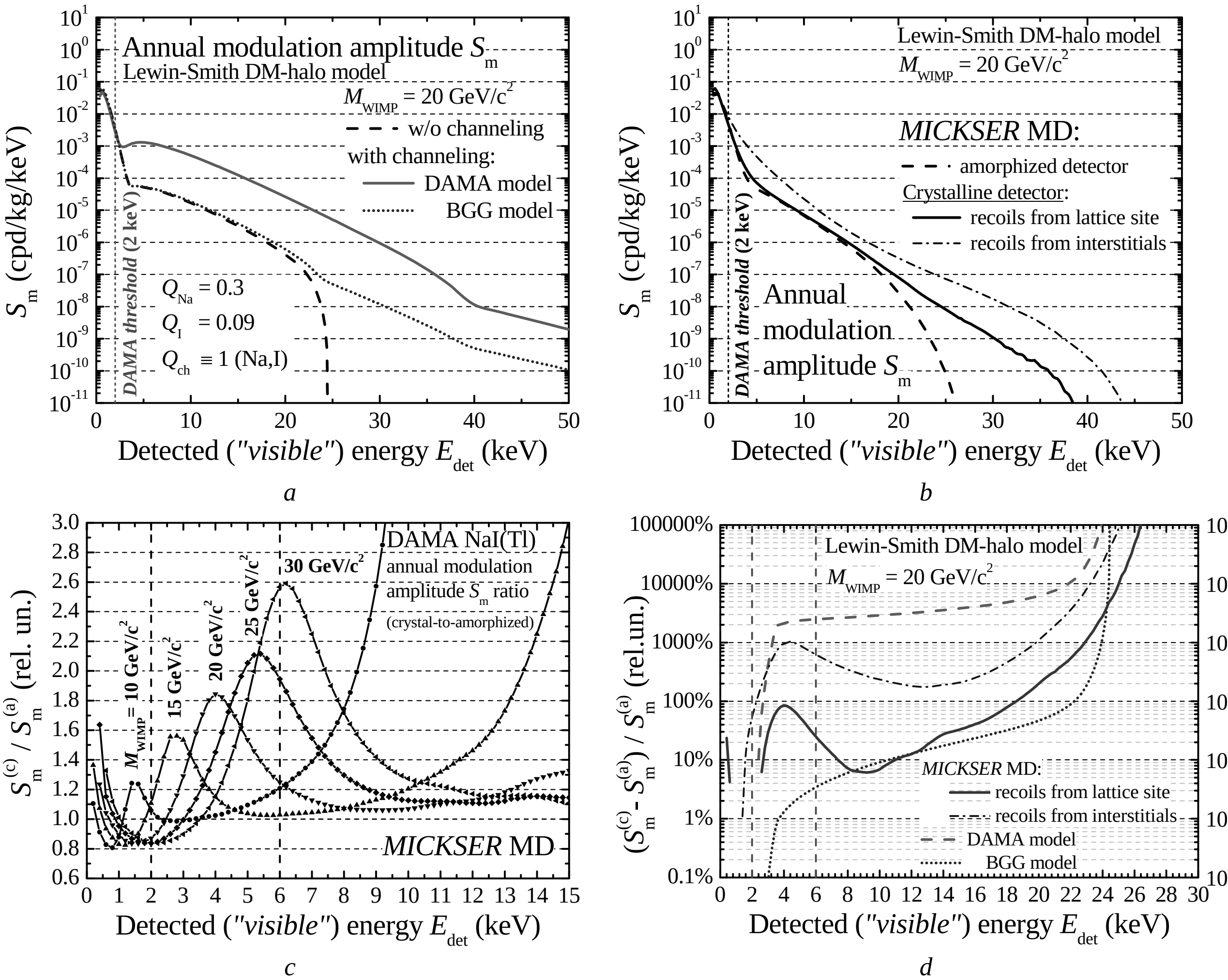


Fig. 7. Absolute (*a* and *b*) and relative (*c* and *d*) representations of modulated visible energy spectra in NaI detector calculated within the scope of existing models [6, 9] (*a* and *d*) and MD simulation of the present work (*b* - *d*).

Numerous ion implantation and radiation damage studies argue that similar tailed distributions are very characteristic for keV energies ions transport and collision cascades in crystals. In our case, their impact on visible energy spectra is notable enough to be included into calibrations and analysis of DM experiments, also for other DMp models and other (CsI, $CaWO_4$, Si, Ge, *etc.*) detectors. It can be done by means of the developed simulation method and computer code, *MICKSER*.

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