Monte Carlo efficiency calculations for N-type high-purity germanium detector

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First, I would like to thank my supervisor Lukáš Závorka for professional leading of this work. Further, I would like to thank my colleagues Martin Suchopár and Radek Vespalec for discussing problems. Last but not least, I thank people from UNC for allowing me to participate in this practice that was very contributive.

1 Introduction

Full energy peak efficiency calibration is one of the most important tasks concerning high-purity germanium (HPGe) detector measurements. There are two major ways of evaluating the efficiency: to measure it experimentally or to use Monte Carlo based simulation programs. However, the simulated efficiency is typically 10-20 % higher than the experimentally measured one [1].

The aim of this work is to computationally simulate the full energy peak efficiency of N-type HPGe detector that is used in YASNAP laboratory for gamma and x-ray spectrometry. The efficiency has already been determined experimentally but not simulated yet. Gaining a reliable mathematical model could be helpful for data evaluation of experiments using this detector. Parallelly to the peak efficiency investigations, also values of total efficiencies were evaluated and briefly discussed.

2 Materials and methods

2.1 Experimental setup

The experimental setup (see figure 1) consists of three main components: detector, shielding and position device. In this section, these components will be described.

Figure 1: Experimental setup.

2.1.1 Detector

The object of interest was n-type high-purity germanium detector (model GR1819). The schematic drawing can be seen in figure 2.

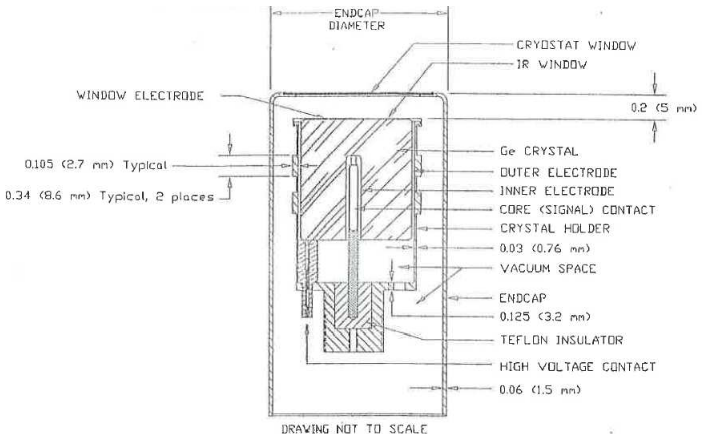

Figure 2: Schematic drawing of N-type HPGe detector.

Detector crystal is made from germanium and can be described by 48 mm in diameter, 49 mm in length, core hole diameter of the crystal is 9 mm and core hole depth is 35 mm. Thickness of the outer electrode (dead outer layer) of the crystal is 0.3 μm and is made from Ge equivalent material. Inner electrode (dead inner layer) thickness is 0.5 mm and made from Ge equivalent material, window electrode thickness is 0.3 μm and made from Ge equivalent material.

Cryostat window of the detector chamber is made from beryllium with thickness of 0.5 mm. Irradiation window consists of two layers. The first one is made from metalized mylar with thickness of 8.47 μm followed by the 101.6 μm kapton layer. Endcap and crystal holder are made from aluminium and encap thickness is 1.5 mm. In the space between detector and detector chamber, vacuum is present. On the top of the detector (cryostat window), 3 mm thick high-density polyethylene (HDPE) cover is placed (not visualised in figure 2).

2.1.2 Shielding

The detector is situated in the shielding box with dimensions: 72 cm in lenght, 55.3 cm in width and 45.9 cm in height. The walls are 7.2 cm thick and are constructed by lead bricks, while the entrance part is missing. In the upper part of the box, there is 1.9 cm dural plate followed by 1 mm copper layer and 1 mm cadmium layer. On the bottom of the box, the lead is followed by 1 mm cadmiun and 1 mm copper layer. The back and side walls are covered by 1 mm cadmium layer.

2.1.3 Position device

The experimantal setup also includes the position device that serves for placing the measured samples (e.g. calibration samples) to defined measuring positions. The position device is made from HDPE and allows to place the samples to the central axis of the detector to the distances from the HDPE cover of: 0.3 cm, 1.1 cm, 1.8 cm, 2.6 cm, 3.6 cm, 4.7 cm, 6.45 cm, 8.2 cm, 10.5 cm, 13.25 cm, 17.2 cm, 21.4 cm, 26.5 cm, 32.9 cm and 40.5 cm.

2.2 Simulations

The simulations were performed in MCNPX (version 2.7) Monte Carlo based computational programme.

According to the data given in section 2.1.1 and 2.1.2, the geometry of the experimental setup (for MCNPX input file) was modeled (see figure 3).

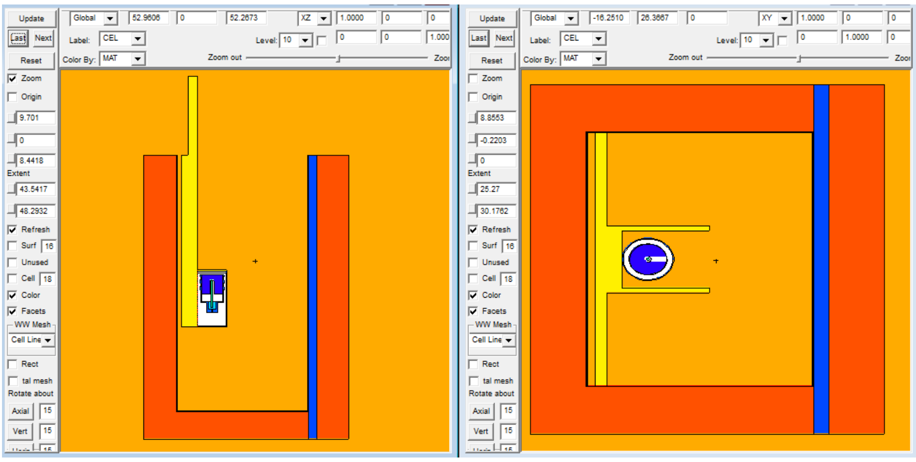

Figure 3: Geometry of experimental setup visualized in MCNPX visual editor Vised (version X_24E).

Unfortunately, a lot of dimensions needed for the geometry model were missing (e.g. endcap diameter), i.e. they were guessed according to the most probable options.

The virtual photon source used for simulations was defined as monoenergetic point source emitting particles into space angle of 4π. It was placed into position 4 (2.6 cm, see section 2.1.3) and the calculations were made for various photon energies: 17.60 keV, 30.97 keV, 59.54 keV, 88.03 keV, 122.06 keV, 165.86 keV, 244.70 keV, 344.28 keV, 443.97 keV, 510.77 keV, 661.66 keV, 785.37 keV, 964.08 keV, 1332.49 keV, 1620.50 keV, 1836.06 keV and 2614.51 keV.

After each simulation, we were given information about spectrum of the energy distribution of pulses created in the detector (Ge crystal) by radiation. From these data, full energy peak efficiency (number of counts in the peak of the emitted energy from the source devided by the total number of particles emitted) and total efficiency (total number of counts in the spectrum of the emitted energy from the source devided by the total number of particles emitted) of the detector were evaluated.

3 Results and discussion

3.1 Peak efficiency

The graphs of resulting peak efficiencies are visible in figure 4.

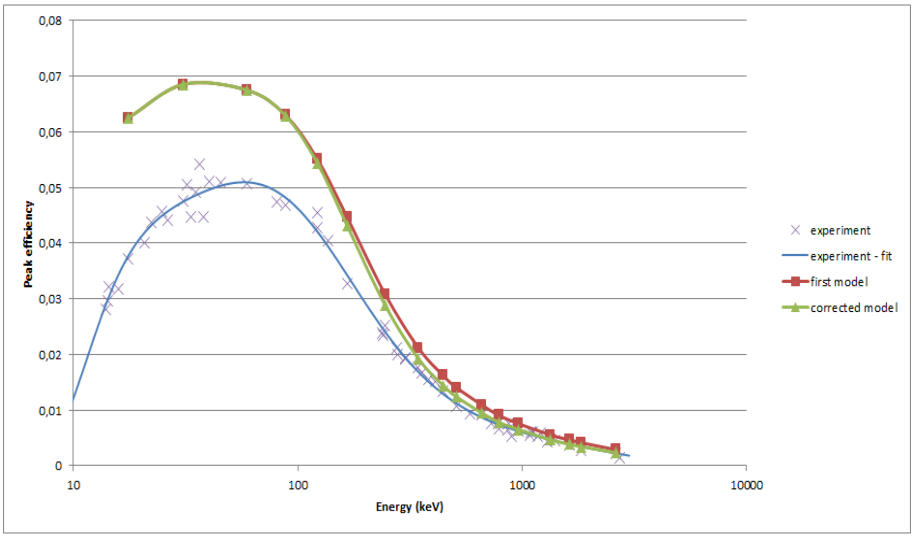

Figure 4: Simulated peak efficiency for first and corrected model of the experimental setup.

In this figure, there are graphs for efficiecies of so called "first model", "second model" and real efficiency (blue line; experimentally measured and fitted by Radek Vespalec). First model efficiency relates to the calculations that were made right after modeling the geometry of the experimental setup and performing the simulations and evaluations as described in section 2.2. Corrected model efficiency relates to such calculations with just model geometry change made in order to get better agreement of simulated and real efficiency.

The agreement is well described by so called R factor (see figure 5). R factor is defined as the ratio of simulated and real peak efficiency for a given photon energy. That means, the closer is the value of R factor to one, the more accurate the simulation is.

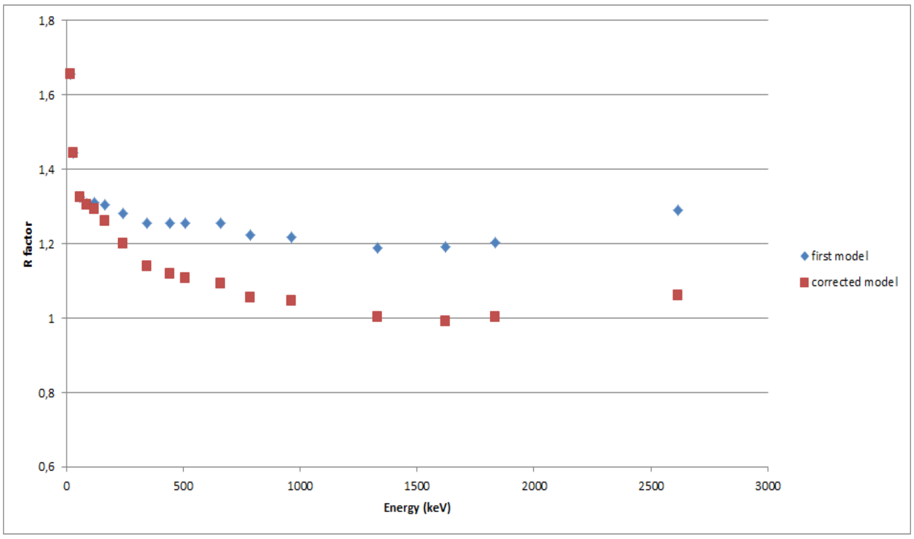

Figure 5: Ratio of simulated and real peak efficiency (R factor) for first and corrected model of the experimental setup.

From the figure, we can observe around 20-30 % disagreement for first model effectivity, while in the region of very low photon energies the discrepancies are even much higher (around 65 % for 17.60 keV). In order to get lower values of R factor, the model geometry of the detector was changed (and the effectivity calculations made again) . The correction was performed in the way of raising the thickness of the inner electrode of the detector (see figure 2) from 0.5 mm to 3.5 mm (part of the Ge crystal was replaced by the electrode). As apparent from the figure 5, good agreement was achieved for higher energies, but the discrepancies in low energy region remained significant (or even did not change for very low photon energies). This result can be explained by the fact that low energy photons are absorbed close to the crystal surface where they enter the crystal, i.e. they can hardly reach the inner electrode and thus the effect of inner electrode thickness rise is minimal (while becomes more considerable with increasing the photon energy).

3.2 Total efficiency

The graphs of resulting total efficiencies and corresponding values of R factor are visible in figures 6 and 7.

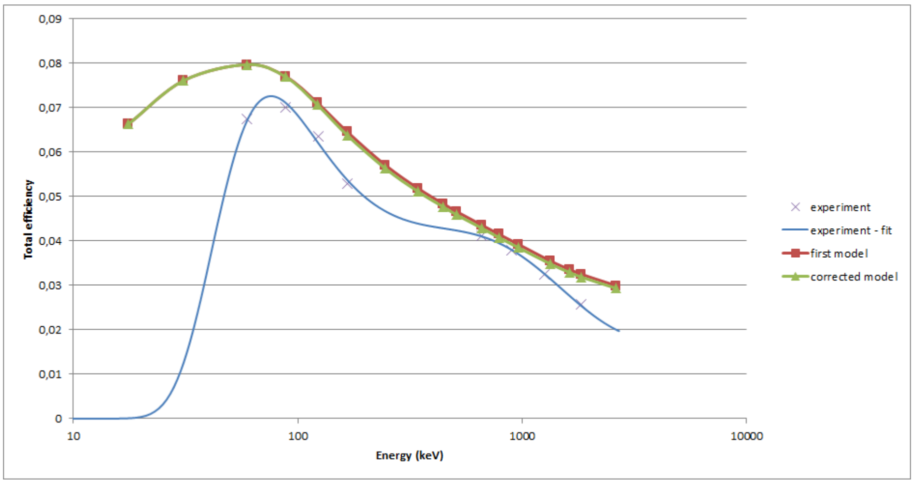

Figure 6: Simulated total efficiency for first and corrected model of the experimental setup.

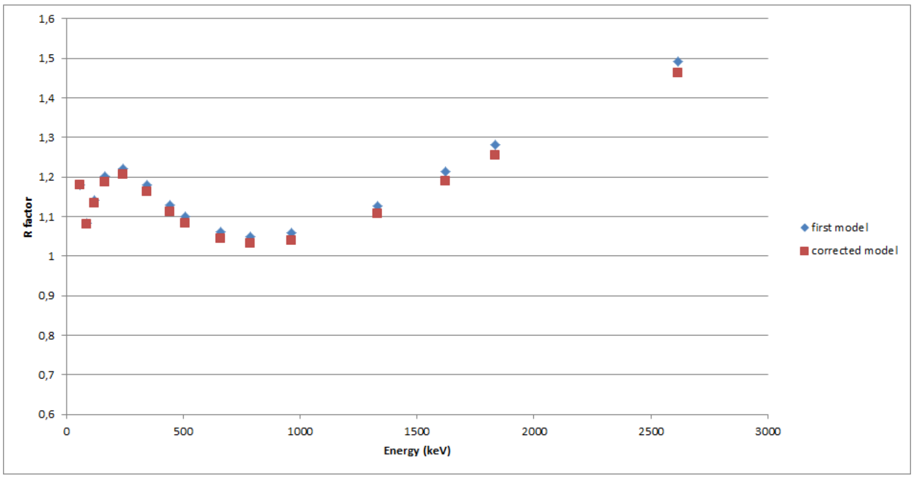

Figure 7: Ratio of simulated and real total efficiency (R factor) for first and corrected model of the experimental setup.

The precision of real total efficiency (experimentally measured and fitted by Radek Vespalec) cannot be considered to be very precise because of low number of experimental measurements (even the very low energy region can be denoted as wrong because of absolute absence of experimental points and cannot be taken as reliable data).

Despite that, we can observe that the effect of correction made in the first model is less obvious compared to the peak efficiency results (figures 4 and 5).

This was expected because the evaluation of the total efficiencies includes sum of the counts of the whole spectrum (measured and simulated) and thus also photons that are less probable to be absorbed in the dead inner layer.

From 7 we can also notice that the correction helped a little to decrease the value of R factor (in comparison with the first model), especially for higher energies. This happened because photons with higher energies are more likely absorbed in the inner electrode.

4 Conclusions

Nevertheless, even if the inner electrode thickness increase helped us to fix the values of full energy peak efficiency for the higher energy region, it does not have to mean that this change is correct. There could exist a lot of free parameters (e.g. cryostat window thickness, outer electrode thickness, IR window material etc.) that could help the model to provide us with more reliable results. Additionally, the reason of differences between simulated and real efficiency does not have to lay in inaccuracies of parameters of such a kind. The discrepancies can also be caused by degradation of dead layers (crystal electrodes) about what is dealt in [1]. Authors of this work also made roentgenographic picture (of similar kind of the detector we used) and discovered that the crystal was rounded on the top. This could also be the cause of differences in simulated and real efficiency we observed and also food for thought for next investigation.

References

1. Boson J., Agren G. and Johansson L., *A detailed investigation of HPGe detector response for improved Monte Carlo efficiency calculations*, Nuclear Instruments and Methods in Physics Research, A 587 (2008) 304–314.

2. Liye L., Jizeng M., Franck D., Carlan L. and Binquan Z., *Monte Carlo efficiency transfer method for full energy peak efficiency calibration of three type HPGe detectors: A coaxial N-type, a coaxial P-type and four BEGe detectors*, Nuclear Instruments and Methods in Physics Research, A 564 (2006) 608–613.

Appendix

example of MCNPX input file (for position 4 and photon energy 510.77 keV)

```
C  Ge DETEKTOR N-TYPU
C  ----------------------------------------------------------------------------
C  Specifikace bunek (teles/objemu) geometrickeho usporadani:
C  (cisloSkupinyBunek,material,hustota,.,geometrie)
   1  1  -5.323         (-3 2 5 -1):(4 -3 -5)  $ zakladni Ge krystal
   2  1  -5.323         (-5 -4 7):(2 -7 -5 6) $ vnitrni elektroda
   20 2 -2.7  (-20 8 -11 21):(-21 22 -20 24):(-22 27 -23 24):(-23 -27 28 25): &
      (-11  29 -26  20): &
     (-26 20 -30  31):(-26 20 -32 33) $ crystal holder
   21 3  -2.250000     (-21  27 -24 50):(-50 -40 27)     $ teflon insulator
   22 4  -8.96           -50 -7  40                    $ core(signal)contact
   3  1  -5.323         (2 -3  1 -8):(-8  3 -9)  $ vnejsi elektroda
   4  7  -1.380000      -8  9 -10  $ okenko krystalu MYLAR
   5  6  -1.420000      -8 10 -11  $ okenko krystalu KAPTON
   70 8  -0.930000      -97 9697 -92 $ VICKO (z HDPE) NAVIC
 7000 9  -0.001205      96 -9697 -92
   90 2  -2.7  (-92 91 -95 93):(-92 91 94 -93):(94 -93 -91) $ obalkaBezVrchnihoOkenka
   91 5  -1.8477              -92 95 -96 $ okno obalky(cryostat window)
   92 0           (21 -2 50 -8):(2 -7 -6 50) $vakuum u krystalu
   93 0    (-29 30 20 -26):(20 -26 -31 32):(20 -26 -33 22):(11 -95 -91): &
           (26 -91 22 -11):(23 -91 -22 28):(-28 93 -91): &
           (-27 28 -25) $ vakuum u krystalu
   98 9  -0.001205 ( (80 -99):(-86 -99): &
        (-801 -99 -80 86):(803 -99 -80 86):(-99 -84 -80 86 801 -803): &
        (-99 82 -80 86 801 -803): &
        (-80 97 -824 820 812 -813):(-94 811 -824 820 812 -813): &
        (-97 94 92 -824 820 812 -813) ) #5000 $ airMeziZbytkemVesmiruAModelem
c STINENI
c 80jeCihlovaObalka-zadniStena,spodekPoDesku,1.bocniStena,2.bocS,predekZaDeskou
   80 10 -11.34     (86 -80 801 -802 -82 84):(86 -87 802 -805 -82 84): &
                    (-80 -805 802 87 84 -85):(-80 -805 802 87 -82 83): &
                    (-803 804 86 -80 -82 84)
   81 12  -2.780000     (-80 86 -804 805 -82 84) $ DURAL deska
c 82jeCu1mmVrstvaPoCihlach-predniStena -V REALU 1.HORNI Cu VRSTVA
   82 4 -8.96 (-805 814 85 -83 -80 87)
c 83jeCd1mmVrstvaPoCu1mmVrstve-predniStena-V REALU 2.HORNI Cd VRSTVA
   83 11 -8.650000 (-814 824 87 -80 85 -83)
c 84jeCd1mmVrstvaPoCihlach-zadniStena-V REALU 1.SPODNI Cd VRSTVA
   84 11 -8.650000 (802 -810 85 -83 -80 87)
c 85jeCu1mmVrstvaPoCd1mmVrstve-zadniStena-V REALU 2.SPODNI Cu VRSTVA
   85 4  -8.96     (810 -820 87 -80 85 -83)
c 86jeCd1mmVrstvaPoCihlach-levaBocniS,pravaBocniS,spodek-V REALU 1.VRSTVA BOKY AZadek
   86 11 -8.650000 (-80 87 -824 820 85 -812):(-80 87 -824 820 -83 813): &
                      (87 -811 820 -824 812 -813)
c 5000 - 1.zavorka je vzdusne plexisklo,2.zavorka je strecha na plexisklu
c kdyzVubecNeuvazujuZlab,3.a4.zavorkaJsouStenyZlabuKtereJdouOdSpodkuVzdusnehoPlexi
  5000  8  -0.930000          (94 -80 812 -813 5001 -5002): &
                              (5004 -5005 5002 -5003 -5006 94): &
          (5007 -5004 -5009 5002 -5006 94):(-5008 5005 -5009 5002 -5006 94)
   99 0             99  $ zbytek vesmiru
C  Povinny oddelovac (prazdna radka):

C  ----------------------------------------------------------------------------
C  Specifikace ploch/povrchu vymezujicich bunky:
   1  cz  2.4   $ vnejsi plocha valcoveho Ge krystalu
   2  pz  0     $ spodni plocha
   3  pz  4.9   $ vrchni plocha
```

```
   4  pz  3.80   $ vrchni plocha otvoru Ge krystalu-ZDE ZMENA - ZE 3.5 na 3.80
   5  cz  0.75  $ valecOtvoruVKrystaluBezTloustkyElektrody-ZDE ZMENA - Z 0.45 na 0.75
   6  cz  0.4   $ valec otvor v krystalu s tloustkou elektrody
   7  pz  3.45  $ plocha elektrody
   8  cz  2.40003 $ valec ohr vnejsi elektrodu(a taky vnitrni valec crystal holderu)
   9  pz  4.90003 $ vrchniPlochaVnejsiElektrody(spodni okenka elektrody)+VRCH HOLDERu
  10  pz  4.900877 $ vrchni plocha okenka elektrody 1 (mylaru)
  11  pz  4.911037 $ vrchni plocha okenka elektrody 2 (kaptonu)
c  crystal holder
  20  cz  2.47603 $ valec ohranicujici vnejsek crystal holderu
  21  pz -1.8     $ prvni z rovina pod nulou
  22  pz -2.12    $ druha z rovina pod nulou
  23  cz  1.28    $ spodni valec holderu
  24  cz  0.77    $ valec kolem teflon insulatoru
  25  cz  0.17    $ valcova dira na spodku drzatka
  26  cz  2.67003 $ valec ohr konce Al vystupku drzatka
  27  pz -3.73    $ spodek teflon insulatoru
  28  pz -4.72    $ spodek holderu
  29  pz  4.54    $ spodek vrchniho Al vystupku
  30  pz  3.57    $ vrch 2. Al vystupku
  31  pz  2.71    $ spodek 2. Al vystupku
  32  pz  1.97    $ vrch 3.(spodni) Al vystupku
  33  pz  1.11    $ spodek 3.(spodni) Al vystupku
c  teflon insulator
  40  pz  -3.29   $ spodek core(signal)contact
c  core (signal) contact
  50  cz   0.2    $ valec
c  51  pz   3.15   $ vrchni plocha core(signal)contactu
c  obalka detektoru
  91  cz  3.2 $ obalka - vnitrni valec
  92  cz  3.35 $ obalka - vnejsi valec
  93  pz  -8.04 $ obalka - vnitrni spodni plocha
  94  pz  -8.18 $ obalka - vnejsi spodni plocha
  95  pz  5.40 $ CRYOSTAT WINDOW - vnitrni plocha
  96  pz  5.45 $ obalka + CRYOSTAT WINDOW - vnejsi vrchni plocha+spodekVICKA
 9697 pz  5.85 $ horni plocha vzduchove vrstvy mezi Be okenkem a vickem
c to vicko co je tam navic a neni ve schematu
  97  pz  6.15 $ vrch VICKA
c zbytek vesmiru
  99  so 200   $ kouleSeStredemVeStreduSouradneSoustavyO r=200
c velka cihlova obalka
  80  pz 35.15   $ vrchniRovinaVrchuCihel(PREDEKvREALU)
  81  pz 27.95   $ spodniRovinaVrchuCihel
  82  py 27.65   $ vnejsi y plocha obalky
  83  py 20.15   $ vnitrni y plocha obalky
  84  py -27.65  $ vnejsi y plocha obalky
  85  py -20.15  $ vnitrni y plocha obalky
  86  pz -36.85  $ vnejsi spodni plocha obalky
  87  pz -29.65  $ vnitrni spodni plocha obalky
  88  py -4      $ plochaProOtvorVKonci OTVOR NEREALIZOVAN
  89  py  4      $ plochaProOtvorVKonci OTVOR NEREALIZOVAN
  801 px -15.25  $ zadniVnejsiPlocha
  802 px -8.05   $ zadniVnitrniPlocha
  803 px 30.65   $ vnejsiPredniStena
  804 px 23.45   $ vnitrniPredniStena(iVnejsekPredniDesky)
  805 px 21.55   $ vnitrekPredniDesky
c Cd 1mm vrstva za cihlama
  810 px -7.95   $ vnitrek zadni Cd vrstvy
  811 pz -29.55  $ vnitrek spodni Cd vrstvy
  812 py -20.05  $ vnitrek leve bocni Cd vrstvy
  813 py  20.05  $ vnitrek prave bocni Cd vrstvy
  814 px  21.45  $ vnitrek predni Cd vrstvy
c Cu 1mm vrstva za Cd 1mm vrstvou
  820 px -7.85   $ vnitrek zadni Cu vrstvy
  821 pz -29.45  $ vnitrek spodni Cu vrstvy
  822 py -19.95  $ vnitrek leve bocni Cu vrstvy
  823 py  19.95  $ vnitrek prave bocni Cu steny
  824 px  21.35  $ vnitrek predni Cu steny
```

```
c Al 1mm vrstva za Cu 1mm vrstvou
  830 px -7.75   $ vnitrek zadni Al vrstvy
  831 pz -29.35  $ vnitrek spodni Al vrstvy
  832 py -19.85  $ vnitrek leve bocni Al vrstvy
  833 py  19.85  $ vnitrek prave bocni Al steny
  834 px  21.25  $ vnitrek predni Al steny
c ZAVERECNE VZDUSNE PLEXISKLO A ZLAB
  5001 px -6.85 $ zacatek vzdusneho plexiskla zleva XZ ve Visedu
  5002 px -5.35 $ konec vzdusneho plexiskla zprava XZ ve Visedu
  5003 px -3.35 $ konec strechy vzdusneho plexiskla
  5004 py -4.5  $ levyBokStrechyVzdusnehoPlexi(KdyzNeuvazujiZlab)AIVnitrniLevyZlabu
  5005 py  4.5  $ pravyBokStrechyVzdusnehoPlexi(KdyzNeuvazujiZlab)AIVnitrniPravyZlabu
  5006 pz  55.15 $ PRESAH ZLABU CO VYLEZA V REALU ZE SOUSTAVY
  5007 py -5.3  $ vnejsi levy bok ZLABU
  5008 py  5.3  $ vnejsi pravy bok ZLABU
  5009 px  8    $ v REALU je to nejhornejsi plocha ZLABU
C  Povinny oddelovac (prazdna radka):

C  ---------------------------------------------------------------------------
C  Zadani datovych vstupu (Data Cards):
  mode p e
  imp:p,e 1 22r 0
C Popis zdroje: POZICE 4
sdef par=2 pos 0 0 8.75 erg = d1
si1 L 0.51077
sp1 D 1
C  Specifikace vystupu (tallies):
f8:p 1
e8 0 1e-5 3.6e-4 8191i 2.94912
ft8  GEB 0.0005 0.0012 0.01
C  Specifikace materialu:
  m1  32000    1         $ Ge (prot.cislo+000)
  m2  13000    1         $ Al
  m3  6000     -0.240183 &
      9000     -0.759818 $ teflon ( Polytetrafluoroethylene PTFE (C2F4)n  )
  m4  29000    1         $ Cu
  m5  4000     1         $ Be
  m6  1000     -0.026362 &
      6000     -0.691133 &
      7000     -0.073270 &
      8000     -0.209235 $ KAPTON-tvoren H,C,N,O
  m7  1000     -0.041960 &
      6000     -0.625016 &
      8000     -0.333024 $ MYLAR-dal jsem:Polyethylene Terephthalate(PET)
  m8  1000     -0.143716 &
      6000     -0.856284 $ HDPE(pouzilJsemPolyethylen(non-borated)zDatabaze)
  m9  6000     -0.000124 &
      7000     -0.755268 &
      8000     -0.231781 &
      18000    -0.012827 $ air-C,N,O,Ar
  m10 82000    1         $ Pb
  m11 48000    1         $ Cd
  m12 12000    -0.015000 &
      13000    -0.927000 &
      14000    -0.002830 &
      22000    -0.000850 &
      24000    -0.000570 &
      25000    -0.006000 &
      26000    -0.002830 &
      29000    -0.043500 &
      30000    -0.001420 $ DURAL-pouzitoZMCNPXDatabazeMaterialu:Aluminium,Alloy2024-O
C  Zadani dalsich parametru ulohy:
prdmp j 1e1 1 j 1e1
  print
nps 1e6
cut:p  j  0.001
```